PHYSICAL REVIEW A VOLUME 25, NUMBER 1 JANUARY 1982

Wigner-Kirkwood expansions

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(Received 30 July 1981)

This paper constructs a general method for obtaining series expansions of the logarithm of the configuration function F. For an N-body quantum system with Hamiltonian H and inverse temperature β, the configuration function is the ratio of the exact to the free coordinate-space heat kernels: $F=\langle \vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle/\langle \vec{x}\,|\,e^{-\beta H_0}\,|\,\vec{x}\,'\rangle$. Expansion of $\ln F$ in Planck's constant h leads to the semiclassical expansion of Wigner and Kirkwood, whereas the series in the variable β provides the high-temperature expansion. By the introduction of an appropriate linked-graph method, it is shown how to obtain explicit formulas for the coefficient functions that enter either of these two series. Further, it is established that the same results can be derived by using the Feynman-Kac path-integral description of the partition function.

I. INTRODUCTION

An N-body quantum system is defined by the Hamiltonian pair (H,H_0). The first Hamiltonian H is the sum of the kinetic-energy operator, all inter-particle potentials and external interactions. The second Hamiltonian H_0 is the free kinetic energy. A basic description of the statistical mechanics of this system is provided by the configuration function, F. Take $\vec{x}$ to be a $3N$-dimensional vector variable that gives the position of the N particles and β to be the inverse temperature of the system, then the configuration function is defined by

$$\langle \vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle=F(\vec{x},\vec{x}\,';\beta)\langle \vec{x}\,|\,e^{-\beta H_0}\,|\,\vec{x}\,'\rangle \ . \tag{1.1}$$

This configuration function contains all information about the statistical system when it is in equilibrium. Since $\langle \vec{x}\,|\,e^{-\beta H_0}\,|\,\vec{x}\,'\rangle$ is given by a simple formula, F determines the coordinate-space matrix elements of $e^{-\beta H}$. From the matrix elements of $e^{-\beta H}$ the canonical ensemble average of every quantum-mechanical observable may be found. This paper studies the asymptotic expansions of the function F and finds explicit expressions for the coefficient functions that arise in these expansions.

Let q be the quantum-scale factor

$$q=\frac{\hbar^2}{2m} , \tag{1.2}$$

where $\hbar$ is the rationalized value of Planck's constant and m is the particle mass. If Δ_x denotes the Laplacian associated with $\vec{x}$, then

$$H_0=-q\Delta_x \ . \tag{1.3}$$

The N-body interaction operator V is given by multiplication with the potential field $v(\vec{x})$. In the simplest cases, $v(\vec{x})$ is the sum of local pair interactions, but may also include three- and four-body interactions, etc., as well as external forces. Our detailed calculations require that $v(\vec{x})$ be a smooth (infinitely differentiable) and a bounded function of $\vec{x}$. The full Hamiltonian is then

$$H=H_0+V \ . \tag{1.4}$$

An important asymptotic expansion is the high-temperature expansion around $\beta\simeq 0$,

$$F(\vec{x},\vec{x}\,';\beta,q)\sim \sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}P_n(\vec{x},\vec{x}\,';q) \ . \tag{1.5}$$

This expansion was examined in a previous paper[1] which we shall refer to as I. Briefly, Perelomov[2] showed it is possible to use the Bloch (or heat) equation implied by $e^{-\beta H}$ to find a recursion relation for the functions P_n. In I, we have extended Perelomov's results and the general formula for P_n for all n was obtained. The coefficient function P_n turns out to be an nth-order polynomial in the interaction $v(\vec{x})$ and an $(n-1)$th-order polynomial in the quantum-scale parameter q. Thus, P_n generates a natural semiclassical expansion. In fact, in asymptotic expansions related to the pair (H,H_0), the functions P_n are ubiquitous. For example, let z be the complex energy appearing in Green's function $G(z)=(H-z)^{-1}$. Then the P_n may be used to expand $\langle \vec{x} \,|\, G(z) \,|\, \vec{x}\,' \rangle$ in the limit $|z| \to \infty$. In this context, the functions P_n are encountered in the one-dimensional problem treated by Gelfand and Dikii[3] and in the three-dimensional problem studied by Buslaev.[4] Furthermore, in the one-dimensional case the $\vec{x}$ integral of the diagonal value $(\vec{x}=\vec{x}\,')$ of P_n constructs the constants of motion of the Korteweg–de Vries equation.[5]

The semiclassical and high-temperature expansion Eq. (1.5) is not suitable in all situations. Since P_n is an nth-order polynomial in v, expansion (1.5) is a perturbation expansion in powers of v. If v is large, then even when $F(\vec{x},\vec{x}\,';\beta,q)$ is dominated by classical N-particle behavior, the series (1.5) will converge very slowly, if at all. This difficulty is removed by summing to all orders the classical terms in the series. This is efficiently done by looking at the exponential forms of (1.5). The two important physical parameters of the system are β and q, so we examine the two series

$$\ln F(\vec{x},\vec{x}\,';\beta,q) \sim \sum_{n=0}^{\infty} q^n S_n(\vec{x},\vec{x}\,';\beta) , \tag{1.6}$$

$$\ln F(\vec{x},\vec{x}\,';\beta,q) \sim \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} W_n(\vec{x},\vec{x}\,';q) . \tag{1.7}$$

The first of these expansions is essentially the Wigner-Kirkwood[6,7] semiclassical expansion. The second series, (1.7), provides one with generating functions for the P_n expansion.

The specific objective of this paper is to find explicit forms of the coefficient functions S_n and W_n. This problem turns out to be more difficult than the construction of the functions P_n. The greater difficulty is easily seen in the nature of the recursion relations for these functions. P_n has a linear recursion relation whereas both S_n and W_n satisfy nonlinear recursion relations. Nevertheless, it will be possible to find the explicit forms of S_n and W_n. The basic idea behind the solution given here is to use perturbation theory in the coupling constant. Take α to be the coupling constant and

$$H_\alpha \equiv H_0 + \alpha V . \tag{1.8}$$

If F_α is the configuration function for the pair (H_α,H_0), then we define

$$\ln F_\alpha(\vec{x},\vec{x}\,';\beta,q) \sim \sum_{n=1}^{\infty} \alpha^n L_n(\vec{x},\vec{x}\,';\beta,q) . \tag{1.9}$$

Setting $\alpha=1$, of course, recovers the original problem (H,H_0). We shall show it is possible to use a linked-graph method to construct L_n. Then, given the series (1.9), one may rearrange it to obtain either (1.6) or (1.7). In the process, one obtains the functions S_n and W_n.

In Sec. II, we derive two different formal representations of F. The first is due to Goldberger and Adams.[8] A formula extracted from the Goldberger-Adams representation will be the point of departure for the construction of the linked-graph form of the functions L_n. The second representation is based on a parametric form of the Hamiltonian and is particularly useful in obtaining the nonlinear recursion relations obeyed by S_n and W_n. Section III constructs the linked-graph solution for series (1.9). In Sec. IV, the functions L_n are restructured so as to obtain formulas for S_n and W_n. Section IV also gives the recursion relations for S_n and W_n. Section V contains an illustration of the theory when it is applied to the n-dimensional harmonic oscillator. The harmonic-oscillator problem is interesting because it has an exact solution for the function F. Thus, S_n and W_n may be obtained directly from their definitions and the formulas compared with predictions of our linked-graph method. Conclusions are found in Sec. VI. The Appendix contains a discussion of our results that is based on a path-integral approach. In particular, we clarify the relationship between the Goldberger-Adams representation and the functional-integral form of F. We show it is a simple matter to pass from the Goldberger-Adams representation of F to that of a path-integral form given in terms of the conditional Wiener measure. It is then shown that the fundamental formula of Sec. II can be obtained from the functional-integral representation of F by purely path-integral techniques.

Most of the mathematical derivations that follow are of an heuristic nature. For example, it is assumed throughout that the expansions (1.5)–(1.9) have meaning and are at least asymptotically convergent series. Further, in a number of places, we assume that integration and summation may be interchanged. The basic purpose of this paper is to find explicit formulas for the coefficient functions W_n and S_n, and in the process to expose the rather elaborate algebraic and combinational structure present in these functions. A rigorous treatment of these unresolved mathematical aspects of the problems raised here is possible, but would involve different language and techniques than are employed in this paper.

II. REPRESENTATIONS OF THE CONFIGURATION FUNCTION

This section derives two useful representations of the configuration function F. The first representation follows from the form of the time-ordered solution of the Schrödinger equation expressed in coordinate space. This solution, first obtained by Goldberger and Adams,[8] is rearranged to find an ordered exponential differential operator form of F. This form provides a convenient starting point for the linked-graph analysis in Sec. III. Our second representation is also an ordered exponential series. It, however, is based on a linear-path parametric form of the Hamiltonian.

In the N-body Hilbert space $e^{-(i/\hbar)H_0 t}$ is the free-particle time-evolution operator. We shall consistently work in the interaction picture. The potential-energy operator in this picture has the definition

$$V_I(t)=V_I^\dagger(t)=e^{+(i/\hbar)H_0 t}Ve^{-(i/\hbar)H_0 t} . \tag{2.1}$$

Here, the dagger denotes the adjoint of an operator. The equation of motion for the exact time-evolution operator $X(t)$ is

$$-i\hbar\frac{d}{dt}X(t)=X(t)V_I(t) , \tag{2.2}$$

and the well-known time-ordered solution is

$$\begin{aligned}X(t)&=e^{+(i/\hbar)Ht}e^{-(i/\hbar)H_0 t}\\ &=\exp_<\left[\frac{i}{\hbar}\int_0^t dt' V_I(t')\right] .\end{aligned} \tag{2.3}$$

The symbol $\exp_<$ denotes the ordered exponential defined by

$$\begin{aligned}\exp_<\left[\frac{i}{\hbar}\int_0^t dt' V_I(t')\right]-1&\equiv\sum_{n=1}^{\infty}\frac{1}{n!}\left[\frac{i}{\hbar}\right]^n\int_0^t\cdots\int_0^t dt_1\cdots dt_n[V_I(t_1)V_I(t_2)\cdots V_I(t_n)]_<\\ &=\sum_{n=1}^{\infty}\left[\frac{i}{\hbar}\right]^n\int_<^t d^n t\, V_I(t_1)V_I(t_2)\cdots V_I(t_n) .\end{aligned} \tag{2.4}$$

The bracket $[\;]_<$ notation means that the operator argument of $[\;]_<$ is a t-ordered product with increasing arguments—the largest t factor appearing on the right. The integral symbol $\int_<^t$ specifies a similar convention

$$\int_<^t d^n t\equiv\int_{0\le t_1\le\cdots\le t_n\le t}\cdots\int dt_1\cdots dt_n . \tag{2.5}$$

The decreasing t-ordered product and its related exponential are represented by $[\;]_>$ and $\exp_>$.

The first step is to transform (2.4) to its β equivalent form realized in coordinate space. Let $t'=\xi t$ and set $t=i\hbar\beta$. Equation (2.3) assumes the form

$$e^{-\beta H}=\exp_<\left[-\beta\int_0^1 d\xi\, e^{-\beta\xi H_0}Ve^{\beta\xi H_0}\right]e^{-\beta H_0} . \tag{2.6}$$

We introduce the following new parameters $\gamma\equiv\beta q$ and $U\equiv\beta V$. Take the coordinate-space Dirac matrix elements of Eq. (2.6) with respect to $\langle\vec{x}\,|$ and $|\,\vec{x}\,'\rangle$. This gives us the kernel form of Eq. (2.6),

$$\begin{aligned}\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle&\\ =\exp_<&\left[-\int_0^1 d\xi\, e^{\gamma\xi\Delta_x}U(\vec{x})e^{-\gamma\xi\Delta_x}\right]\\ &\times\langle\vec{x}\,|\,e^{-\beta H_0}\,|\,\vec{x}\,'\rangle .\end{aligned} \tag{2.7}$$

The configuration function F is the ratio of $\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle$ to $\langle\vec{x}\,|\,e^{-\beta H_0}\,|\,\vec{x}\,'\rangle$. Thus, Eq. (2.7) is not suitable as it stands to express F. To remedy this, move the expression $\langle\vec{x}\,|\,e^{-\beta H_0}\,|\,\vec{x}\,'\rangle$ through all the operators in $\exp_<$. Assume g to be any analytic function of $\vec{x}$, which admits a Taylor series expansion about 0. According to the relationship

$$e^{s\Delta_x}\vec{x}\,e^{-s\Delta_x}=\vec{x}+2s\vec{\nabla}_x \tag{2.8}$$

we get

$$e^{s\Delta_x}g(\vec{x})e^{-s\Delta_x}=g(\vec{x}+2s\vec{\nabla}_x) , \tag{2.9}$$

for any scalar s. With this differential operator notation, Eq. (2.7) reads

$$\begin{aligned}\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle=\exp_<&\left[-\int_0^1 d\xi\, U(\vec{x}+2\gamma\xi\vec{\nabla}_x)\right]\\ &\times\langle\vec{x}\,|\,e^{-\beta H_0}\,|\,\vec{x}\,'\rangle .\end{aligned} \tag{2.10}$$

Examine, for the moment, the explicit form of $\langle \vec{x} \,|\, e^{-\beta H_0} \,|\, \vec{x}\,' \rangle$. Let 2δ be the dimension of $\vec{x}$. The function $\langle \vec{x} \,|\, e^{-\beta H_0} \,|\, \vec{x}\,' \rangle$ is the free-particle solution of the heat equation

$$\langle \vec{x} \,|\, e^{-\beta H_0} \,|\, \vec{x}\,' \rangle = \frac{1}{(4\pi\gamma)^\delta} e^{-(\vec{x}-\vec{x}\,')^2/4\gamma} . \tag{2.11}$$

Using

$$e^{[(\vec{x}-\vec{x}\,')^2/4\gamma]} \vec{\nabla}_x e^{-(\vec{x}-\vec{x}\,')^2/4\gamma} = \vec{\nabla}_x - \frac{1}{2\gamma}(\vec{x}-\vec{x}\,') , \tag{2.12}$$

it is a simple matter to verify that

$$U(\vec{x}+2\gamma\xi\vec{\nabla}_x)e^{-(\vec{x}-\vec{x}\,')^2/4\gamma} = e^{[-(\vec{x}-\vec{x}\,')^2/4\gamma]} U(\vec{x}+\xi(\vec{x}\,'-\vec{x})+2\gamma\xi\vec{\nabla}_x) . \tag{2.13}$$

Identity (2.13), when combined with (2.10), gives us the Goldberger-Adams representation

$$F(\vec{x},\vec{x}\,';\gamma) = \exp_< \left[-\int_0^1 d\xi\, U(\hat{\xi}+2\gamma\xi\vec{\nabla}_x) \right] 1 . \tag{2.14}$$

In Eq. (2.14), we employ the linear-path notation

$$\hat{\xi} \equiv \vec{x}+\xi(\vec{x}\,'-\vec{x}) , \quad \xi\in[0,1] . \tag{2.15}$$

For $\xi=0$, the initial point of the path is $\vec{x}$. The final point for $\xi=1$ is at $\vec{x}\,'$. This type of linear path will appear again and again in our analysis. The 1, which occurs to the right of $\exp_<$ in Eq. (2.14), is the function of $\vec{x}$ with constant value 1.

Although the Goldberger-Adams relation (2.14) gives an explicit and exact representation of $F(\vec{x},\vec{x}\,';\gamma)$, its limitations are apparent. The series in $\exp_<$ is complicated by the ordering process. Further, the integrand $U(\hat{\xi}+2\gamma\xi\vec{\nabla}_x)$ is difficult to work with because of the $\vec{\nabla}_x$ in the argument. We now alter Eq. (2.14) in order to make its algebraic structure more transparent. Note first that since $\langle \vec{x} \,|\, e^{-\beta H} \,|\, \vec{x}\,' \rangle$ and $\langle \vec{x} \,|\, e^{-\beta H_0} \,|\, \vec{x}\,' \rangle$ are left invariant by the the interchange $\vec{x}\leftrightarrow\vec{x}\,'$, then $F(\vec{x},\vec{x}\,';\gamma)=F(\vec{x}\,',\vec{x};\gamma)$. This symmetry implies Eq. (2.14) can be written

$$F(\vec{x},\vec{x}\,';\gamma) = \exp_< \left[-\int_0^1 d\xi' U(\check{\xi}'+2\gamma\xi'\vec{\nabla}_{x'}) \right] 1 . \tag{2.16}$$

Here $\check{\xi}$ represents the path which is the transpose of $\hat{\xi}$,

$$\check{\xi} \equiv \vec{x}\,'+\xi(\vec{x}-\vec{x}\,') , \quad \xi\in[0,1] . \tag{2.17}$$

Change the variables ξ_i' in Eq. (2.16) by the substitution

$$\xi_i' = 1-\xi_{n+1-i} \quad (i=1\sim n) . \tag{2.18}$$

In particular, note that

$$\begin{aligned} \check{\xi}_1' &= \vec{x}\,'+\xi_1'(\vec{x}-\vec{x}\,') \\ &= \vec{x}\,'+(1-\xi_n)(\vec{x}-\vec{x}\,') = \hat{\xi}_n . \end{aligned} \tag{2.19}$$

Further, this change of variables (2.18) preserves the ordering process, i.e., $0\le\xi_1'\le\xi_2'\cdots\le\xi_n'\le1$ becomes $0\le\xi_1\le\xi_2\cdots\le\xi_n\le1$. Thus, the nth term in the $\exp_<$ expansion of (2.16) becomes

$$(-1)^n \int_<^1 d^n\xi\, U(\hat{\xi}_n+2\gamma(1-\xi_n)\vec{\nabla}_{x'}) \cdots U(\hat{\xi}_1+2\gamma(1-\xi_1)\vec{\nabla}_{x'})1 . \tag{2.20}$$

Equation (2.9) permits us to write the integrand of (2.20) as

$$\begin{aligned} J \equiv{} & \exp[\gamma(1-\xi_n)\xi_n^{-1}\Delta_{x'}]U(\hat{\xi}_n)\exp[-\gamma(1-\xi_n)\xi_n^{-1}\Delta_{x'}] \\ & \times\exp[\gamma(1-\xi_{n-1})\xi_{n-1}^{-1}\Delta_{x'}]U(\hat{\xi}_{n-1})\cdots\exp[\gamma(1-\xi_1)\xi_1^{-1}\Delta_{x'}]U(\hat{\xi}_1) . \end{aligned} \tag{2.21}$$

In order to simplify the gradient and Laplacian structure here, define $\vec{\nabla}_i$ by

$$\vec{\nabla}_i U(\hat{\xi}_j) \equiv \delta_{ij}(\vec{\nabla}U)(\hat{\xi}_j) . \tag{2.22}$$

The right-hand side of (2.22) is to be interpreted as letting $\vec{\nabla}_x$ act on $U(x)$, after that putting $\vec{x}=\hat{\xi}_j$. Gradient $\vec{\nabla}_i$ acts on only the factor U having argument $\hat{\xi}_i$. An advantage of $\vec{\nabla}_i$ is that the commutator $[\vec{\nabla}_i,\vec{\nabla}_j]=0$ for all i, j. In terms of $\vec{\nabla}_i$, we can write

$$\Delta_{x'}\prod_{i=1}^{l}U(\hat{\xi}_i)=\left[\sum_{i=1}^{l}\xi_i\vec{\nabla}_i\right]^2\prod_{i=1}^{l}U(\hat{\xi}_i)\quad (l=1\sim n)\ . \tag{2.23}$$

The integrand J is now expressed by

$$J=\exp\left[\gamma(1-\xi_n)\xi_n^{-1}\left[\sum_{i=1}^{n}\xi_i\vec{\nabla}_i\right]^2\right]U(\hat{\xi}_n)\exp\left[-\gamma(1-\xi_n)\xi_n^{-1}\left[\sum_{i=1}^{n-1}\xi_i\vec{\nabla}_i\right]^2\right]$$
$$\times\exp\left[\gamma(1-\xi_{n-1})\xi_{n-1}^{-1}\left[\sum_{i=1}^{n-1}\xi_i\vec{\nabla}_i\right]^2\right]U(\hat{\xi}_{n-1})\cdots\exp[\gamma(1-\xi_1)\xi_1^{-1}(\xi_1\vec{\nabla}_1)^2]U(\hat{\xi}_1)\ . \tag{2.24}$$

The potential functions $U(\hat{\xi}_i)$ may be moved to the right. Because of the commutivity properties of the $\vec{\nabla}_i$, the operator arguments of the exponentials can be combined, giving

$$J=\exp\left[\beta q\sum_{l=1}^{n}\sum_{i=1}^{n}\phi(\xi_l,\xi_i)\vec{\nabla}_l\cdot\vec{\nabla}_i\right]U(\hat{\xi}_1)\cdots U(\hat{\xi}_n)\ , \tag{2.25}$$

where the function ϕ is defined in terms of $\xi_<\equiv\min\{\xi,\xi'\}$ and $\xi_>\equiv\max\{\xi,\xi'\}$ by

$$\phi(\xi,\xi')\equiv\xi_<(1-\xi_>)\ . \tag{2.26}$$

Finally we obtain, after putting $U=\beta V$, the representation

$$F(\vec{x},\vec{x}\,';\beta,q)=\sum_{n=0}^{\infty}(-\beta)^n\int_<^1 d^n\xi\exp\left[\beta q\sum_{l,i=1}^{n}\phi(\xi_l,\xi_i)\vec{\nabla}_l\cdot\vec{\nabla}_i\right]v(\hat{\xi}_1)\cdots v(\hat{\xi}_n)\ . \tag{2.27}$$

Formula (2.27) is the principal result of this section. It is from here that the derivation of the linked-graph representation begins. One immediate application of Eq. (2.27) is to construct the formula for the coefficient functions $P_n(\vec{x},\vec{x}\,';q)$ which enter the β expansion of F, Eq. (1.5). By expanding the exponential of Eq. (2.27) in a series with respect to the variable β we can identify the total coefficient of β^m and in this way find $P_m(\vec{x},\vec{x}\,';q)$. This yields the expressions for $P_m(\vec{x},\vec{x}\,';q)$, found in I.[9]

We will now turn our attention to a second representation of F. In the following, $\vec{x}\,'$ and q are taken as fixed constants, so we suppress their appearance in F, i.e., $F(\vec{x};\beta)=F(\vec{x},\vec{x}\,';\beta,q)$. The heat equation for $\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle$ is

$$\left[\frac{\partial}{\partial\beta}+H\right]\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle=0\ . \tag{2.28}$$

Here $\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle$ denotes the solution of Eq. (2.28) that satisfies the boundary condition

$$\lim_{\beta\to0}\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle=\delta(\vec{x}-\vec{x}\,')\ . \tag{2.29}$$

The partial differential equation satisfied by F is obtained by substituting definition (1.1) into Eq. (2.28):

$$\left[\frac{\partial}{\partial\beta}+\frac{1}{\beta}(\vec{x}-\vec{x}\,')\cdot\vec{\nabla}_x-q\Delta_x+v(\vec{x})\right]F(\vec{x};\beta)=0\ . \tag{2.30}$$

Now introduce the linear path in $\vec{x}$ space parametrized by a constant $\beta_0>0$,

$$\tilde{x}(\vec{x},\beta\beta_0^{-1})=\vec{x}\,'+\beta\beta_0^{-1}(\vec{x}-\vec{x}\,')\ ,\quad 0\le\beta\le\beta_0\ . \tag{2.31}$$

This path has extreme points $\tilde{x}(\vec{x},0)=\vec{x}\,'$, $\tilde{x}(\vec{x},1)=\vec{x}$. Take $g=g(\vec{x};\beta)$ to be any function of $(\vec{x},\beta)$. Then the total derivative with respect to β is

$$\frac{d}{d\beta}g(\tilde{x}(\vec{x},\beta\beta_0^{-1});\beta)=\left[\frac{\partial}{\partial\beta}+\frac{1}{\beta}(\tilde{x}-\vec{x}\,')\cdot\vec{\nabla}_{\tilde{x}}\right]g(\tilde{x};\beta)\ . \tag{2.32}$$

Note that in writing the second factor in the large parentheses we have used the identity $(\tilde{x}-\vec{x}\,')\beta^{-1}=(\vec{x}-\vec{x}\,')\beta_0^{-1}$. We omit the arguments of path $\tilde{x}$ whenever there is no ambiguity in the notation. Consider the effect of H on a path-dependent function $g(\tilde{x}(\vec{x},\beta\beta_0^{-1});\beta)$. Set

$$H(\tilde{x})\equiv-q\Delta_{\tilde{x}}+v(\tilde{x})\ , \tag{2.33}$$

then

$$(Hg)(\tilde{x})=H(\tilde{x})g(\tilde{x};\beta)\ . \tag{2.34}$$

With identities (2.32) and (2.34), we see that

$$\left[\frac{d}{d\beta}+H(\tilde{x})\right]F(\tilde{x};\beta)=0\ , \tag{2.35}$$

is equivalent to

$$\left[\frac{\partial}{\partial\beta}+\frac{1}{\beta}(\tilde{x}-\vec{x}\,')\cdot\vec{\nabla}_{\tilde{x}}-q\Delta_{\tilde{x}}+v(\tilde{x})\right]F(\tilde{x};\beta)=0\ . \tag{2.36}$$

In this fashion the partial differential Eq. (2.30) is reduced to a form, (2.35), that permits integration with respect to β.

It is evident that $F(\tilde{x},\beta)$ satisfies the integral equation

$$F(\tilde{x},\beta)=1-\int_0^\beta d\beta' H(\tilde{x}(\vec{x},\beta'\beta_0^{-1}))\times F(\tilde{x}(\vec{x},\beta'\beta_0^{-1});\beta')\ . \tag{2.37}$$

This integral equation incorporates the boundary condition corresponding to Eq. (2.29), namely, $F(\tilde{x};0)=1$. Changing variables to $\xi=\beta\beta_0^{-1}$ and $\xi_1=\beta'\beta_0^{-1}$, then letting $\beta_0\to\beta$ and $\xi=1$ gives us

$$F(\vec{x};\beta)=1-\beta\int_0^1 d\xi_1 H(\tilde{x}(\vec{x},\xi_1))\times F(\tilde{x}(\vec{x},\xi_1);\xi_1\beta)\ . \tag{2.38}$$

To clarify the content of the parameteric integral equation, it suffices to examine its behavior under iteration. Replace $\vec{x}\to\tilde{x}(\vec{x},\xi_1)$ and $\beta\to\xi_1\beta$ in Eq. (2.38), then

$$F(\tilde{x}(\vec{x},\xi_1);\xi_1\beta)=1-\xi_1\beta\int_0^1 d\xi_2 H(\tilde{x}(\tilde{x}(\vec{x},\xi_1),\xi_2))F(\tilde{x}(\tilde{x}(\vec{x},\xi_1),\xi_2);\xi_1\xi_2\beta)\ . \tag{2.39}$$

Now the algebraic structure of (2.31) for $\tilde{x}$ implies the composition rule

$$\tilde{x}(\tilde{x}(\vec{x},\xi_1),\xi_2)=\tilde{x}(\vec{x},\xi_1\xi_2)\ . \tag{2.40}$$

The combination of (2.38) and (2.39) gives us the first iterated integral equation

$$F(\vec{x};\beta)=1-\beta\int_0^1 d\xi_1 H(\tilde{x}(\vec{x},\xi_1))1+\beta^2\int_0^1 \xi_1 d\xi_1\int_0^1 d\xi_2 H(\tilde{x}(\vec{x},\xi_1))H(\tilde{x}(\vec{x},\xi_1\xi_2))F(\tilde{x}(\vec{x},\xi_1\xi_2);\xi_1\xi_2\beta)\ . \tag{2.41}$$

Finally, change the variables ξ_1,ξ_2 by the substitution $\xi_1'=\xi_1$ and $\xi_2'=\xi_1\xi_2$, then (2.41) becomes

$$F(\vec{x};\beta)=1-\beta\int_0^1 d\xi_1' H(\tilde{x}(\vec{x},\xi_1'))1+\beta^2\int_0^1 d\xi_1'\int_0^{\xi_1'} d\xi_2' H(\tilde{x}(\vec{x},\xi_1'))H(\tilde{x}(\vec{x},\xi_2'))F(\tilde{x}(\vec{x},\xi_2');\xi_2'\beta)\ . \tag{2.42}$$

In this fashion, it is seen that the general iteration sums to give the ordered exponential

$$F(\vec{x},\vec{x}\,';\beta,q)=\exp_>\left[-\beta\int_0^1 d\xi\, H(\tilde{x}(\vec{x},\xi))\right]1\ . \tag{2.43}$$

One measure of the utility of representation (2.43) is the ease with which it can be used to obtain recursion relations. Consider expansion (1.5) of F in powers of β. Clearly,

$$P_n(\vec{x},\vec{x}\,';q)=n!\int_>^1 d^n\xi\, H(\tilde{x}(\vec{x},\xi_1))\cdots H(\tilde{x}(\vec{x},\xi_n))1\ . \tag{2.44}$$

If the change of the parameters ξ_i is made to restore their range of variation to [0,1], then an immediate consequence of (2.44) is

$$P_n(\vec{x},\vec{x}\,';q)=n\int_0^1 d\xi\,\xi^{n-1}H(\tilde{x}(\vec{x},\xi))P_{n-1}(\tilde{x}(\vec{x},\xi),\vec{x}\,';q)\ . \tag{2.45}$$

This is Perelomov's recursion relation[2] for $P_n(\vec{x},\vec{x}\,';q)$ [Eq. (2.19) of I]. What Eq. (2.43) shows us is that by introducing the linear parametric path, Eq. (2.31), we have been able to obtain the exponentiation of the recursion relations (2.45).

III. LINKED-GRAPH EXPANSION OF ln$F$

This section analyzes the consequences of representation (2.27). By finding the appropriate symmetry in the parameters ξ_i, we show how the ξ ordering may be removed. Then a set of operator definitions is found that allows one to write the series (2.27) in such a way that its nth term has the same combinational structure as possessed by the linked-cluster expansion in classical statistical mechanics. The graphical description of the terms in Eq. (2.27) will permit us to explicitly exponentiate the series and thus arrive at the expansion of $\ln F$ in the coupling-constant parameter.

Each v in expansion (2.27) carries one power of α. So the F_α defined by the Hamiltonian pair (H_α, H_0) can be expressed as

$$F_\alpha(\vec{x},\vec{x}\,';\beta,q)=\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}Z_n(\vec{x},\vec{x}\,';\beta,q)\ , \tag{3.1}$$

where $Z_n(\vec{x},\vec{x}\,';\beta,q)$ is defined as follows: Let $\vec{\xi}=(\xi_1,\xi_2,\ldots,\xi_n)$, and

$$f_k(\vec{x},\vec{x}\,';\beta,\xi_k)\equiv-\beta\{\exp[\beta q(1-\xi_k)\xi_k\Delta_k]\}v(\hat{\xi}_k)\ , \tag{3.2}$$

$$\mathscr{F}_n(\vec{\xi})\equiv\prod_{k=1}^{n}f_k(\vec{x},\vec{x}\,';\beta,\xi_k)\ . \tag{3.3}$$

With this notation Z_n is given by

$$Z_n(\vec{x},\vec{x}\,';\beta,q)=n!\int_<^1 d^n\xi\exp\left[2\beta q\sum_{j=2}^{n}\sum_{i=1}^{j-1}\xi_i(1-\xi_j)\vec{\nabla}_i\cdot\vec{\nabla}_j\right]\mathscr{F}_n(\vec{\xi})\ . \tag{3.4}$$

This form of Z_n emerges because all the diagonal terms of the exponential argument of Eq. (2.27)—those where $l=i$ and which lead to a Laplacian $\vec{\nabla}_l\cdot\vec{\nabla}_l=\Delta_l$—are incorporated in the definition of the $f_l(\vec{x},\vec{x}\,';\beta,\xi_l)$. The remaining portion of the exponential argument consists of the off-diagonal scalar products $\vec{\nabla}_i\cdot\vec{\nabla}_j$, $i\neq j$, that couple two different f_k to each other.

Consider a symmetrization of the integrand of Z_n that permits us to eliminate the ξ-ordering restriction in (3.4). For any pair of integers i and j let $\xi_<=\min(\xi_i,\xi_j)$ and $\xi_>=\max(\xi_i,\xi_j)$. Define the operator $a_{ij}(\vec{\xi})$ by

$$a_{ij}(\vec{\xi})\equiv\begin{cases}\exp[2\beta q\xi_<(1-\xi_>)\vec{\nabla}_i\cdot\vec{\nabla}_j]-1\ , & i\neq j\\ 0, & i=j\ .\end{cases} \tag{3.5}$$

For all $\vec{\xi}$ belonging to the unit n-dimensional cube $Q\equiv[0,1]^n$, these operators have the following obvious properties:

$$a_{ij}(\vec{\xi})=a_{ji}(\vec{\xi})\ , \tag{3.6}$$

$$[a_{ij}(\vec{\xi}),a_{kl}(\vec{\xi})]=0\ . \tag{3.7}$$

In particular, if $i<j$ and $\xi_i\leq\xi_j$ then

$$a_{ij}(\vec{\xi})=\exp[2\beta q\xi_i(1-\xi_j)\vec{\nabla}_i\cdot\vec{\nabla}_j]-1\ . \tag{3.8}$$

Let $\mathscr{I}_n(\vec{\xi})$ denote the exponential operator occurring in the integrand of Z_n. With the $a_{ij}(\vec{\xi})$ this may be written

$$\mathscr{I}_n(\vec{\xi})\equiv\prod_{j=2}^{n}\prod_{i=1}^{j-1}[1+a_{ij}(\vec{\xi})]\ . \tag{3.9}$$

Consider the symmetry of $\mathscr{I}_n(\xi_1,\xi_2,\ldots,\xi_n)$ under an arbitrary permutation of the labels $1,2,\ldots,n$. The form (3.8) of $a_{ij}(\vec{\xi})$ permits us to define a square root by

$$[a_{ij}(\vec{\xi})+1]^{1/2}\equiv\begin{cases}\exp[\beta q\xi_<(1-\xi_>)\vec{\nabla}_i\cdot\vec{\nabla}_j]\ , & i\neq j\\ 1\ , & i=j\ .\end{cases} \tag{3.10}$$

Keeping in mind the commutivity $[\vec{\nabla}_i\cdot\vec{\nabla}_j, \vec{\nabla}_k\cdot\vec{\nabla}_l]=0$, we see that $\mathscr{I}_n(\vec{\xi})$ can be expressed

$$\mathscr{I}_n(\vec{\xi})=\prod_{j=1}^{n}\prod_{i=1}^{n}[1+a_{ij}(\vec{\xi})]^{1/2}\ . \tag{3.11}$$

The right-hand side of (3.11) is obviously invariant under any permutation of $1,2,\ldots,n$. The definition (3.3) of $\mathscr{F}_n(\vec{\xi})$ implies the $\mathscr{F}_n(\vec{\xi})$ also shares this permutation invariance. So the complete integrand of Z_n, $\mathscr{I}_n(\vec{\xi})\mathscr{F}_n(\vec{\xi})$, is invariant. Thus we have

$$n!\int_<^1 d^n\xi\,\mathscr{I}_n(\vec{\xi})\mathscr{F}_n(\vec{\xi})=\int_0^1\cdots\int_0^1 d\xi_1\cdots d\xi_n\mathscr{I}_n(\vec{\xi})\mathscr{F}_n(\vec{\xi})\ . \tag{3.12}$$

Having removed the ξ-ordered aspect of Z_n, it is possible to see the way in which the graphical enumeration problem arises in Z_n. Introduce the somewhat artificial notation

$$\int df_i\equiv\int_0^1 d\xi_i f_i(\vec{x},\vec{x}\,';\beta,\xi_i)\ . \tag{3.13}$$

Then Z_n reads

$$Z_n(\vec{x},\vec{x}\,';\beta,q)=\int\cdots\int\prod_{i<j}^{n}[1+a_{ij}(\vec{\xi})]\times df_1\cdots df_n\ . \tag{3.14}$$

It is apparent that the integral (3.14) has precisely the same combinatorial structure as one encounters in the fugacity expansion of the classical grand canonical partition function. The variable in the problem here corresponding to the fugacity is the coupling constant α.[10] Thus it is reasonable to expect that we can achieve an exponentiation of the series (3.1) that is analogous to the exponentiation of the fugacity expansion of the grand partition function via the linked-cluster expansion.

Consider the graphical description of the term Z_n. Expanding the product $\prod_{i<j}^{n}$ gives $\frac{1}{2}n(n-1)$ separate integrals whose sum is Z_n. Each integral is associated with an n-vertex graph. An n-vertex graph consists of n separate vertices (or sites)—each vertex identified uniquely by one of the labels $i=1\sim n$. A vertex with label i represents the function $f_i(\vec{x},\vec{x}\,';\beta,\xi_i)$. A link between vertices i and j denotes the presence of the operator $a_{ij}(\vec{\xi})$ in the integral. Between each pair of vertices there is at most one link.

For example, one integral, G_{10}, in the sum that defines Z_{10} is

$$G_{10}\equiv\int\cdots\int a_{12}a_{39}a_{67}a_{68}a_{6,10}a_{78}df_1\cdots df_{10}\ . \tag{3.15}$$

This integral is represented by the graph of Fig. 1. Integrals like G_{10} simplify because they factor, viz.,

$$G_{10}=\left[\int df_4\right]\left[\int df_5\right]\left[\int\int a_{12}df_1df_2\right]\times\left[\int\int a_{39}df_3df_9\right]\times\left[\int\cdots\int a_{67}a_{68}a_{6,10}a_{78}df_6df_7df_8df_{10}\right]. \tag{3.16}$$

Note this factorization is only possible because we have removed the ξ-ordering structure in the original form of Z_n. Define an l-vertex linked graph as a graph in which the links form at least one unbroken pathway connecting each vertex to every other vertex. The factorization property of G_n is that each graph is characterized by a product of linked graphs. Let m_l be the recurrence frequency of the l-vertex linked graphs in G_n. So G_n defines the set $\{m_l\}$ where $\{m_l\}$ is subject to the constraint

$$\sum_{l=0}^{n} lm_l=n\ . \tag{3.17}$$

Next decompose the Z_n sum of graphs G_n into two stages. First, let

$$Z_n(\vec{x},\vec{x}\,';\beta,q)=\sum_{\{m_l\}}S\{m_l\} \tag{3.18}$$

where

$$S\{m_l\}=\sum \text{all } G_n \text{ consistent with } \{m_l\}\ . \tag{3.19}$$

Finally, define a cluster integral L_l to be the sum of all possible distinct l-vertex linked graphs times $l!^{-1}$. For example, the first three L_l are given by

$$L_1(\vec{x},\vec{x}\,';\beta,q)=\int df_1\ , \tag{3.20}$$

$$L_2(\vec{x},\vec{x}\,';\beta,q)=\frac{1}{2!}\int\int a_{12}df_1df_2\ , \tag{3.21}$$

$$L_3(\vec{x},\vec{x}\,';\beta,q)=\frac{1}{3!}\int\int\int(a_{12}a_{13}+a_{12}a_{23}+a_{13}a_{23}+a_{12}a_{13}a_{23})\times df_1df_2df_3\ . \tag{3.22}$$

The graph enumeration problem encountered here is identical with that which occurs in representation of the classical partition function for a system whose total potential energy is a sum of pairwise local potentials. The well-known[10] solution of this graph counting problem is

$$S\{m_l\}=\frac{n!}{m_1!m_2!\cdots m_l!}\times(L_1)^{m_1}(L_2)^{m_2}(L_3)^{m_3}\cdots(L_l)^{m_l}\ . \tag{3.23}$$

Substituting Eqs. (3.23), (3.19), and (3.18) into (3.1) gives us

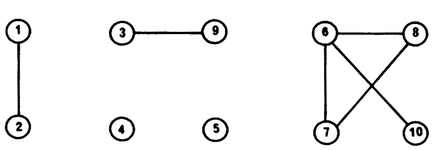

FIG. 1. The graph G_{10}.

$$F_\alpha(\vec{x},\vec{x}\,';\beta,q)=\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}\sum_{\{m_l\}}\frac{n!}{m_1!m_2!\cdots m_l!}(L_1)^{m_1}\cdots(L_l)^{m_l}$$

$$=\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\cdots\sum_{m_l=0}^{\infty}\frac{(\alpha L_1)^{m_1}}{m_1!}\frac{(\alpha^2 L_2)^{m_2}}{m_2!}\cdots\frac{(\alpha^l L_l)^{m_l}}{m_l!}\cdots . \tag{3.24}$$

Thus we arrive at

$$F_\alpha(\vec{x},\vec{x}\,';\beta,q)=\exp\left[\sum_{l=1}^{\infty}\alpha^l L_l(\vec{x},\vec{x}\,';\beta,q)\right], \tag{3.25}$$

which is equivalent to Eq. (1.9). The linked-cluster expansion (3.25) embodies a major restructuring of the differential forms appearing in Eq. (2.27). Since f_i is formed by an exponential of a Laplacian acting on $v(\hat{\xi})$, the series (3.25) involves a twofold exponentiation of Δ_i.

Our final task is to work out how the series (3.25) implies the functional form of the expansions of $\ln F$ in powers of either β or q. We introduce several new operators that will assist in exposing the β,q dependence. Set

$$b_{ij}(\vec{\xi})\equiv\xi_<(1-\xi_>)\vec{\nabla}_i\cdot\vec{\nabla}_j , \tag{3.26}$$

$$c_n(\vec{\xi})\equiv\sum_{i=1}^{n}(1-\xi_i)\xi_i\Delta_i , \tag{3.27}$$

$$v_i\equiv v(\hat{\xi}_i) . \tag{3.28}$$

In terms of the b_{ij}, we can write a_{ij} as the series

$$a_{ij}(\vec{\xi})=\sum_{l_{ij}\geq 1}\frac{(2\beta q)^{l_{ij}}}{l_{ij}!}b_{ij}^{l_{ij}}(\vec{\xi}) . \tag{3.29}$$

Consider the linked cluster L_n. It has a maximum of $\frac{1}{2}n(n-1)$ links. Let s be the sum of all possible $\frac{1}{2}n(n-1)$ values of l_{ij}, i.e.,

$$s\equiv\sum_{i>j}^{n}l_{ij} . \tag{3.30}$$

Using this notation L_n assumes its final form

$$L_n(\vec{x},\vec{x}\,';\beta,q)=\sum_{\mathscr{G}_n}\frac{(-1)^n 2^s}{n!m!}\beta^{n+m+s}q^{m+s}$$
$$\times\int d^n\xi\prod_{i>j}^{n}\frac{b_{ij}^{l_{ij}}}{l_{ij}!}c_n^m v_1 v_2\cdots v_n . \tag{3.31}$$

This is a consequence of inserting the operators b_{ij}, c_n, and the function v_i into the form of the general l-vertex linked graph that enters the definition of L_n. The operators c_n come from the product of the arguments $\beta q(1-\xi_k)\xi_k\Delta_k$ in the exponential formula (3.2) for f_k. The summation convention in (3.31) is such that m always goes from 0 to ∞.

The graphical structure of an arbitrary l cluster is absorbed in the definition of the summation convention denoted by $\mathscr{G}_n$. Consider first the case $n=3$. The allowed l_{ij} are $\{l_{12},l_{13},l_{23}\}$. Then the l_{ij} part of the sum in (3.31) is

$$\sum_{\mathscr{G}_3}=\sum_{l_{12}\geq 1}\sum_{l_{13}\geq 1}+\sum_{l_{12}\geq 1}\sum_{l_{23}\geq 1}+\sum_{l_{13}\geq 1}\sum_{l_{23}\geq 1}$$
$$+\sum_{l_{12}\geq 1}\sum_{l_{13}\geq 1}\sum_{l_{23}\geq 1} , \tag{3.32}$$

where it is understood for the first term on the right-hand side, one sets $l_{23}=0$ inside the integrand of (3.31). Likewise, for the second and third terms $l_{13}=0$ and $l_{12}=0$, respectively. The summation convention for $\mathscr{G}_n$ is the obvious generalization of the $n=3$ case. Setting aside the m summation which is always present, the $\mathscr{G}_n$ sum has as many distinct sums over the l_{ij} as there are distinct connected graphs in L_n. The distinct sums are constructed by the following procedure. Start first with the maximally connected n-vertex graph having $\frac{1}{2}n(n-1)$ links. The sum for this graph has all $l_{ij}\geq 1$. Next consider all graphs formed from the first one by removing one link. If the link between i and j is removed, then set $l_{ij}=0$. In this way, one forms all possible $\frac{1}{2}n(n-1)$ linked graphs having exactly $\frac{1}{2}n(n-1)-1$ links. Next remove two links and set the corresponding values of $l_{ij}=0$. If this process is continued, subject to the constraint that the graphs formed this way remain connected, one forms all possible graphs in L_n. Note that the minimum number of links consistent with a connected graph is $n-1$. Thus $s\geq n-1$. In the $\mathscr{G}_4$ vertex case, the six links $\{l_{12},l_{13},l_{14},l_{23},l_{24},l_{34}\}$ have one graph with six links, six graphs with five links, fifteen graphs with four links, and sixteen graphs with three links. This gives a total of 38 connected graphs. As n increases this graph structure becomes formidably complex. The number[11] of connected graphs with $n=5$, 6, and 7 are, respectively, 728, 26 704, and 1 866 256.

Equation (3.31) provides us with an explicit construction of the linked-graph function L_n. This formula and its companion Eq. (3.25) are the basic results of this paper. Since the β and q dependence are manifest in Eq. (3.31), it is a simple matter to construct the β and q power-series expansions of $\ln F$.

IV. COEFFICIENT FUNCTIONS S_n AND W_n

In this section, we transform the linked-cluster expansion of $\ln F$ into a practical computational method for obtaining the functions $S_n(\vec{x},\vec{x}\,';\beta)$ and $W_n(\vec{x},\vec{x}\,';q)$. Formulas for both on- and off-diagonal values of the functions S_n and W_n are derived. This section illustrates the fact that the linked-graph expansion, Eqs. (3.25) and (3.31), contains all other expansions of $\ln F$. At the end of this section we obtain the recursion relations satisfied by S_n and W_n.

Consider the behavior of the first three linked-cluster terms L_1, L_2, and L_3. Equation (3.31) for $n=1,2,3$ assumes the form

$$L_1=-\sum \frac{1}{m!}\beta^{1+m}q^m \int_0^1 d\xi_1 c_1^m v_1 , \tag{4.1}$$

$$L_2=\sum \frac{2^s}{2!m!}\beta^{2+m+s}q^{m+s} \times \int_0^1 \int_0^1 d\xi_1 d\xi_2 \frac{1}{l_{12}!} b_{12}^{l_{12}} c_2^m v_1 v_2 , \tag{4.2}$$

$$L_3=-\sum \frac{2^s}{3!m!}\beta^{3+m+s}q^{m+s} \times \int_0^1 \int_0^1 \int_0^1 d\xi_1 d\xi_2 d\xi_3 \frac{b_{12}^{l_{12}} b_{13}^{l_{13}} b_{23}^{l_{23}}}{l_{12}!l_{13}!l_{23}!} c_3^m v_1 v_2 v_3 , \tag{4.3}$$

where the argument of L_n is $(\vec{x},\vec{x}\,';\beta,q)$ and $\sum$ has the $\mathscr{G}_n$ summation convention. Observe that the lowest power of β in L_n is $2n-1$ and that the lowest power of q is $n-1$. So if we have constructed $\{L_1,L_2,L_3\}$, we can obtain the functional forms of $\{W_1,W_2,W_3,W_4,W_5,W_6\}$ and $\{S_0,S_1,S_2\}$. In this way the L_n become efficient generators of the functions W_n and S_n.

Let us examine the Wigner-Kirkwood expansion in detail. The series (1.6) is equivalent to

$$F=\exp S_0 \exp(qS_1+q^2S_2+q^3S_3+q^4S_4+\cdots) \tag{4.4}$$

$$=\exp S_0[1+qS_1+q^2(S_2+\tfrac{1}{2}S_1^2)+q^3(S_3+S_1S_2+\tfrac{1}{6}S_1^3)+q^4(S_4+S_1S_3+\tfrac{1}{2}S_2^2+\tfrac{1}{2}S_2S_1^2+\tfrac{1}{24}S_1^4)+\cdots] . \tag{4.5}$$

In Eq. (4.5), we have used the cummulant formulas[12] to expand the second exponential as a series in the quantum-scale parameter q. The form (4.5) is the expansion appearing in the work of Wigner[6] and Kirkwood.[7] The term S_0 is the sum of all terms in the exponential of (3.25) that have power q^0. Because the minimum power of q in L_n is $n-1$, the only linked cluster with q^0 is L_1. From (4.1), we see that the q^0 component of L_1 is just

$$S_0(\vec{x},\vec{x}\,';\beta)=-\beta \int_0^1 d\xi_1 v_1 . \tag{4.6}$$

Turning to S_1, we see that the $m=1$ component of L_1 has q power equal to one and so also does the $m=0$, $l_{12}=1$ portion of L_2. No other L_n contributes, so

$$S_1(\vec{x},\vec{x}\,';\beta,q)=-\beta^2 \int_0^1 d\xi_1 c_1 v_1+\beta^3 \int_0^1 \int_0^1 d\xi_1 d\xi_2 b_{12} v_1 v_2 . \tag{4.7}$$

With S_2, the L_1 contribution is $m=2$; the L_2 contribution is $m=0$, $l_{12}=2$ and $m=1, l_{12}=1$ and finally L_3 contributes with $m=0$, $l_{12}=l_{13}=1$, etc. Thus S_2 is

$$S_2(\vec{x},\vec{x}\,';\beta)=-\tfrac{1}{2}\beta^3 \int_0^1 d\xi_1 c_1^2 v_1+\beta^4 \int_0^1 \int_0^1 d\xi_1 d\xi_2 (b_{12}c_2+b_{12}^2) v_1 v_2 -\tfrac{2}{3}\beta^5 \int_0^1 \int_0^1 \int_0^1 d\xi_1 d\xi_2 d\xi_3 (b_{12}b_{13}+b_{12}b_{23}+b_{13}b_{23}) v_1 v_2 v_3 . \tag{4.8}$$

Continuing this process constructs all S_n. One of the reasons why the linked-cluster series for $\ln F$ is a practical method of constructing S_n is that although the L_n are very complicated functions, the coefficient functions S_n and W_n use only a few of the infinite number of terms defining the L_n. The formulas (4.6)–(4.8) still involve one parametric integration of the linear paths $\hat{\xi}_i$. Without special assumption on v these integrals cannot be simplified further.

Expansion (4.5) and the formula for $S_n(\vec{x},\vec{x}\,';\beta)$ generalize the original Wigner-Kirkwood analysis in that we have kept the full off-diagonal form of the matrix elements. Thus, one can incorporate the exchange effects that are a consequence of fermion or boson statistics. In the classical limit $q\to 0$, the $\vec{x}\simeq\vec{x}\,'$ region of the matrix element $\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle$ dominates, so let us consider the behavior of the diagonal values of S_n. Here $\vec{x}=\vec{x}\,'$ implies

$$v_i=v(\hat{\xi}_i)=v(\vec{x})\ . \tag{4.9}$$

This means there is no ξ dependence in the potential arguments in formula for the S_n. So the v_i may be taken out of the integrations in Eqs. (4.6)–(4.8). The S_0 is trivial:

$$S_0(\vec{x},\vec{x};\beta)=-\beta v(\vec{x})\ . \tag{4.10}$$

The S_1 is typical of the diagonal evaluation of S_n. For $\vec{x}=\vec{x}\,'$, Eq. (4.7) can be written

$$S_1=-\beta^2(\Delta v)\int_0^1 d\xi_1(1-\xi_1)\xi_1 +\beta^3(\vec{\nabla}_1\cdot\vec{\nabla}_2)v_1v_2\int_0^1\int_0^1 d\xi_1 d\xi_2\xi_<(1-\xi_>)\ . \tag{4.11}$$

The ξ_i integrals are always polynomials of ξ_i and can be explicitly carried out. Here one finds

$$S_1(\vec{x},\vec{x};\beta)=-\tfrac{1}{6}\beta^2\Delta v(\vec{x})+\tfrac{1}{12}\beta^3[\vec{\nabla}v(\vec{x})]^2\ . \tag{4.12}$$

In a similar fashion the value of S_2 is found to be

$$S_2(\vec{x},\vec{x};\beta)=-\tfrac{1}{60}\beta^3(\Delta^2 v)+\beta^4[\tfrac{1}{30}(\vec{\nabla}\Delta v)\cdot\vec{\nabla}v+\tfrac{1}{90}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2 v_1v_2]-\tfrac{1}{60}\beta^5(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_1\cdot\vec{\nabla}_3)v_1v_2v_3\ . \tag{4.13}$$

These expressions are consistent with known[13] forms of the diagonal values of S_n. The $\vec{\nabla}_i$ gradient notation may be eliminated if desired by use of the identities

$$(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_1\cdot\vec{\nabla}_3)v_1v_2v_3=\tfrac{1}{2}\vec{\nabla}v\cdot\vec{\nabla}(\vec{\nabla}v)^2\ , \tag{4.14}$$

$$(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2 v_1v_2=-\vec{\nabla}v\cdot\vec{\nabla}(\Delta v)+\tfrac{1}{2}\Delta(\vec{\nabla}v)^2\ . \tag{4.15}$$

Turn now to the computation of the functions W_n. The method is the same as that just used to determine the S_n. Specifically for a given value of β^n, one collects from the relevant L_l the terms with β-power dependence equal to n. Formulas (1.5) and (1.7) mean W_n and P_n are related by the cummulant identities[12]

$$\begin{aligned}
&P_1=W_1\ ,\quad P_2=W_2+W_1^2\ ,\\
&P_3=W_3+3W_2W_1+W_1^3\ ,\\
&P_4=W_4+4W_3W_1+3W_2^2+6W_2W_1^2+W_1^4\ ,\\
&P_5=W_5+5W_4W_1+10W_3W_2+10W_3W_1^2\\
&\qquad+15W_2^2W_1+10W_2W_1^3+W_1^5\ .
\end{aligned} \tag{4.16}$$

Thus, given the values of $W_1,W_2,\ldots,W_n$, we can construct the P_n. In this way, we can view the W_n as generating functions for P_n. This is a useful point of view since the W_n turn out to be much simpler functions than the corresponding P_n.

The off-diagonal values of the first five W_n are

$$W_1=\int_0^1 d\xi_1 v_1\ , \tag{4.17}$$

$$\frac{1}{2!}W_2=-q\int_0^1 d\xi_1 c_1 v_1\ , \tag{4.18}$$

$$\frac{1}{3!}W_3=q^2\int_0^1 d\xi_1\frac{1}{2!}c_1^2 v_1-q\int_0^1\int_0^1 d\xi_1 d\xi_2 b_{12}v_1v_2\ , \tag{4.19}$$

$$\frac{1}{4!}W_4=-q^3\int_0^1 d\xi_1\frac{1}{3!}c_1^3 v_1+q^2\int_0^1\int_0^1 d\xi_1 d\xi_2(b_{12}^2+b_{12}c_2)v_1v_2\ , \tag{4.20}$$

$$\frac{1}{5!}W_5=q^4\int_0^1 d\xi_1\frac{1}{4!}c_1^4 v_1-q^3\int_0^1\int_0^1 d\xi_1 d\xi_2(\tfrac{2}{3}b_{12}^3+b_{12}^2c_2+\tfrac{1}{2}b_{12}c_2^2)v_1v_2$$
$$+q^2\int_0^1\int_0^1\int_0^1 d\xi_1 d\xi_2 d\xi_3\tfrac{2}{3}(b_{12}b_{13}+b_{12}b_{23}+b_{13}b_{23})v_1v_2v_3 \ . \qquad (4.21)$$

Note that the maximum number of potentials v in the product of the integrands for W_n is $[(n+1)/2]$, where [ ] is the largest integer less than or equal to the argument of [ ]. The maximum power of q in W_n is $n-1$, and the least power of q is $n-[(n+1)/2]$.

The diagonal values of the W_n result from Eqs. (4.17)–(4.21) by setting $\vec{x}=\vec{x}\,'$. The remaining ξ_i integrations are all simple polynomials whose form is given by the definitions (3.26) and (3.27) of b_{ij} and c_n. In this way, one determines that

$$W_1(\vec{x},\vec{x};q)=v(\vec{x}) \ , \qquad (4.22)$$

$$W_2(\vec{x},\vec{x};q)=-q\tfrac{1}{3}\Delta v \ , \qquad (4.23)$$

$$W_3(\vec{x},\vec{x};q)=-q\tfrac{1}{2}(\vec{\nabla}v)^2+q^2\tfrac{1}{10}\Delta^2 v \ , \qquad (4.24)$$

$$W_4(\vec{x},\vec{x};q)=q^2[\tfrac{4}{15}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2v_1v_2+\tfrac{4}{5}(\vec{\nabla}\Delta v)\cdot\vec{\nabla}v]-q^3\tfrac{1}{35}\Delta^3 v \ , \qquad (4.25)$$

$$W_5(\vec{x},\vec{x};q)=q^2 2(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_1\cdot\vec{\nabla}_3)v_1v_2v_3-q^3\{\tfrac{1}{7}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^3v_1v_2+\tfrac{4}{7}(\vec{\nabla}_1\cdot\vec{\nabla}_2)^2(\Delta v_1)v_2$$
$$+\tfrac{3}{7}\vec{\nabla}v\cdot\vec{\nabla}(\Delta^2 v)+\tfrac{17}{42}[\vec{\nabla}(\Delta v)]^2\}+q^4\tfrac{1}{126}\Delta^4 v \ . \qquad (4.26)$$

The formulas quoted above should be compared to those for P_n given in I. For example, P_4 has eight terms whereas W_4 has only three. This is illustrative of the greater simplicity of W_n relative to P_n.

An additional perspective on the functions S_n and W_n is found from the recursion relations these functions satisfy. Define $W\equiv\ln F$, then Eq. (2.35) reads

$$\left[\frac{d}{d\beta}+H(\vec{x}(\vec{x},\beta\beta_0^{-1}))\right]\exp W(\vec{x}(\vec{x},\beta\beta_0^{-1}),\vec{x}\,';\beta)=0 \ . \qquad (4.27)$$

Let $\xi=\beta\beta_0^{-1}$. Then set $\beta_0\to\beta$. Thus the linear path becomes $\vec{x}=\vec{x}(\vec{x},\xi)=\vec{x}\,'+\xi(\vec{x}-\vec{x}\,')$, and Eq. (4.27) is transformed into

$$\left[\frac{d}{d\xi}-q\beta\Delta_{\vec{x}}\right]W(\vec{x},\vec{x}\,';\xi\beta)-q\beta[\vec{\nabla}_{\vec{x}}W(\vec{x},\vec{x}\,';\xi\beta)]^2+\beta v(\vec{x})=0 \ . \qquad (4.28)$$

The coefficients W_n provide the power-series expansion of W via Eq. (1.7). Inserting series (1.7) into (4.28) and equating the total coefficient of the common power of β gives us

$$\frac{d}{d\xi}W_1(\vec{x},\vec{x}\,';q)=v(\vec{x}) \ , \qquad (4.29)$$

$$\frac{1}{2!}\frac{d}{d\xi}W_2(\vec{x},\vec{x}\,';q)=-q\Delta_{\vec{x}}W_1(\vec{x},\vec{x}\,';q) \ . \qquad (4.30)$$

For $n\geq 3$ then

$$\frac{d}{d\xi}W_n(\vec{x},\vec{x}\,';q)=-nq\Delta_{\vec{x}}W_{n-1}(\vec{x},\vec{x}\,';q)-q\sum_{m=1}^{n-2}\frac{n!}{m!(n-1-m)!}\vec{\nabla}_{\vec{x}}W_{n-1-m}(\vec{x},\vec{x}\,';q)\cdot\vec{\nabla}_{\vec{x}}W_m(\vec{x},\vec{x}\,';q) \ . \qquad (4.31)$$

The identities (4.29) through (4.31) provide us with the recursion relations for W_n. These relations are nonlinear and indicate in part why determining the W_n was a more difficult task than finding values for P_n.

If $\exp W$ is expanded by powers of q instead of β, then substituting Eq. (1.6) into (4.28) provides us with the recursion relation for the Wigner-Kirkwood functions S_n,

$$\frac{d}{d\xi}S_0(\vec{x},\vec{x}\,';\xi\beta)=-\beta v(\vec{x}) \ . \qquad (4.32)$$

For $n\geq 1$ then

$$\frac{d}{d\xi}S_n(\vec{x},\vec{x}\,';\xi\beta)=\beta\Delta_{\vec{x}}S_{n-1}(\vec{x},\vec{x}\,';\xi\beta)+\beta\sum_{m=0}^{n-1}\vec{\nabla}_{\vec{x}}S_{n-1-m}(\vec{x},\vec{x}\,';\xi\beta)\cdot\vec{\nabla}_{\vec{x}}S_m(\vec{x},\vec{x}\,';\xi\beta) \ . \qquad (4.33)$$

Although one can construct S_n and W_n from these nonlinear recursion relations, the role of these recursion relations assumes a diminished importance since we have found an explicit algebraic method to form the functions S_n and W_n.

V. THE HARMONIC OSCILLATOR

The basic results of this paper are the formulas given in Secs. III and IV, which construct the coefficient functions for $\ln F(\vec{x},\vec{x}\,';\beta,q)$. The expressions found are quite general and valid for any smooth potential. Nevertheless, it is useful to examine a problem possessing an exact solution in which it is possible to find closed expressions for the coefficient functions L_n, S_n, and W_n. The $3N$-dimensional harmonic oscillator provides us with just such an exactly solvable example. The closed algebraic formulas for L_n, S_n, and W_n, which arise from the harmonic-oscillator problem, can be compared with the predictions of the general theory in Secs. III and IV and so give us an independent check on the validity of our linked-graph solutions.

The Hamiltonian for the $3N$-dimensional harmonic oscillator with common mass m and frequency ω can be written as the sum

$$H_\alpha=\sum_{\nu=1}^{3N} h_\nu \ , \tag{5.1}$$

where

$$h_\nu=-q\frac{\partial^2}{\partial x_\nu^2}+\alpha\tfrac{1}{2}m\omega^2 x_\nu^2 \ . \tag{5.2}$$

Here x_ν denotes one of the $3N$ Cartesian components of the vector $\vec{x}$ and α is a parameter for the potential strength. The one-dimensional problem has the following well-known[14] exact solution. Set $\gamma=\beta q$, $\theta=\hbar\omega\beta$, and $y=\alpha^{1/2}\theta$. With this notation, the one-dimensional heat kernel is

$$\langle x_\nu \,|\, e^{-\beta h_\nu} \,|\, x_\nu' \rangle=\left[\frac{y}{4\pi\gamma \sinh y}\right]^{1/2} \times\exp\left[\frac{-1}{4\gamma}[(x_\nu^2+x_\nu'^2)y\coth y - 2x_\nu x_\nu' y \,\mathrm{csch} y]\right] . \tag{5.3}$$

Because the individual component Hamiltonians h_ν all commute with each other, the solution to the $3N$-dimensional heat kernel is the product of the individual component solutions

$$\langle \vec{x} \,|\, e^{-\beta H} \,|\, \vec{x}\,' \rangle=\sum_{\nu=1}^{3N} \langle x_\nu \,|\, e^{-\beta h_\nu} \,|\, x_\nu' \rangle \ . \tag{5.4}$$

Thus the exact solution for F is

$$F_\alpha(\vec{x},\vec{x}\,';\beta,q)=\left[\frac{y}{\sinh y}\right]^{3N/2}\exp\left[\frac{-1}{4\gamma}[(\vec{x}^{\,2}+\vec{x}\,'^2)(y\coth y-1)-2\vec{x}\cdot\vec{x}\,'(y\,\mathrm{csch} y-1)]\right] , \tag{5.5}$$

where the scalar product $\vec{x}\cdot\vec{x}\,'$ is the sum over $\nu=1\sim 3N$ of $x_\nu x_\nu'$. Taking the logarithm of Eq. (5.5) gives us

$$W_\alpha(\vec{x},\vec{x}\,';\beta,q)=\frac{-1}{4\gamma}[(\vec{x}^{\,2}+\vec{x}\,'^2)(y\coth y-1) -2\vec{x}\cdot\vec{x}\,'(y\,\mathrm{csch} y-1)] -\tfrac{3}{2}N\ln\frac{\sinh y}{y} \ . \tag{5.6}$$

A short calculation allows one to verify that Eq. (5.6) is a solution to the nonlinear equation satisfied by W_α, namely,

$$\left[\frac{\partial}{\partial\beta}+\frac{1}{\beta}(\vec{x}-\vec{x}\,')\cdot\vec{\nabla}_x-q\Delta_x\right]W_\alpha(\vec{x},\vec{x}\,';\beta,q) -q[\vec{\nabla}_x W_\alpha(\vec{x},\vec{x}\,';\beta,q)]^2+\alpha\tfrac{1}{2}m\omega^2\vec{x}^{\,2}=0 \ . \tag{5.7}$$

Furthermore, the boundary condition $W_\alpha(\vec{x},\vec{x}\,';0,q)=0$ is obeyed.

Let us obtain the coupling-constant expansion of W_α in powers of α. The three hyperbolic functions appearing in Eq. (5.6) have the following convergent series expansions[15] for $|y|<\pi$. Let B_{2n} denote the Bernoulli numbers given by the convention

$$B_{2n}\equiv\frac{(-1)^{n-1}2(2n)!}{(2\pi)^{2n}}\sum_{k=1}^{\infty}\frac{1}{k^{2n}} \quad \text{for } n\geq 1 \ , \tag{5.8}$$

and $B_0=1$, then

$$y\coth y-1=\sum_{n=1}^{\infty}B_{2n}\frac{2^{2n}}{(2n)!}y^{2n} \ , \tag{5.9}$$

$$y\,\mathrm{csch} y-1=-2\sum_{n=1}^{\infty}B_{2n}\frac{2^{2n-1}-1}{(2n)!}y^{2n} \ , \tag{5.10}$$

$$\ln\frac{\sinh y}{y}=\sum_{n=1}^{\infty}B_{2n}\frac{2^{2n-1}}{n(2n)!}y^{2n}\ . \qquad (5.11)$$

Inserting these series into Eq. (5.6) gives us the exact series development of W_α,

$$W_\alpha(\vec{x},\vec{x}\,';\beta,q)=\sum_{l=1}^{\infty}\alpha^l L_l(\vec{x},\vec{x}\,';\beta,q)\ , \qquad (5.12)$$

where L_l is

$$L_l(\vec{x},\vec{x}\,';\beta,q)=-B_{2l}\frac{\theta^{2l}}{2\gamma(2l)!}\left[2^{2l-1}(\vec{x}+\vec{x}\,')^2-2\vec{x}\cdot\vec{x}\,'+\frac{3N\gamma}{l}2^{2l-1}\right]. \qquad (5.13)$$

Because the hyperbolic functions (5.9)–(5.11) have convergent series for $|y|<\pi$, it follows that the coupling-constant series is uniformly convergent for all bounded x,x' if $\alpha^{1/2}<\pi/\hbar\omega\beta$. So if the temperature is sufficiently high, then the coupling-constant series is always convergent for any value of α.

The harmonic-oscillator problem is exceptional in that it is possible to find a closed form for the lth-order cluster integral L_l. Let us compare briefly the structure of Eq. (5.13) and the general form of L_l given by the cluster integral Eqs. (3.20)–(3.22). The function f_k, defined by Eq. (3.2), normally is a series in β from β^1 to β^∞. However, since $v(\vec{x})$ is quadratic in $\vec{x}$, only the terms β^1 and β^2 are nonvanishing. Thus, f_k is quadratic in the path variable $\hat{\xi}_n$. The linked graphs in L_l all have $f_1(\hat{\xi}_1)f_2(\hat{\xi}_2)\cdots f_l(\hat{\xi}_l)$ as part of their integrands. This product factor is a polynomial of order $2l$ in the variable x. However, the minimum number of links in an l-vertex connected graph is $(l-1)$ and each has two differentials in the variable x. Thus after the derivatives in the a_{ij} act on the product $f_1(\hat{\xi}_1)\cdots f_l(\hat{\xi}_l)$, one recovers the quadratic $\vec{x}$ dependence shown in formula (5.13).

Consider the functional forms taken on by W_n and S_n. Identifying the β^n power in Eqs. (5.12) and (5.13) gives

$$W_{2n-1}(\vec{x},\vec{x}\,';q)=B_{2n}\frac{(2m)^n}{8n}\omega^{2n}q^{n-1}\times[(\vec{x}^2+\vec{x}\,'^2)2^{2n}+4\vec{x}\cdot\vec{x}\,'(2^{n-1}-1)]\ , \qquad (5.14)$$

$$W_{2n}(\vec{x},\vec{x}\,';q)=-B_{2n}3N\frac{2^{2n-1}}{2n}(2m)^n\omega^{2n}q^n\ . \qquad (5.15)$$

The first formula here provides the value of W_n for odd values of its index; the second formula gives the even index values. Observe that these formulas for W_n only have the terms with the lowest possible power of q. Similarly, examining the coefficient of the q^n power in series (5.12) leads to S_n,

$$S_n(\vec{x},\vec{x}\,';\beta)=-B_{2n+2}\frac{1}{4(2n+2)!}(2m)^{n+1}\omega^{2n+2}\beta^{2n+1}\times[2^{2(n+1)}(\vec{x}^2+\vec{x}\,'^2)+4(2^{2n+1}-1)\vec{x}\,'\cdot\vec{x}]-B_{2n}3N\frac{2^{2n-1}}{2n(2n)!}(2m)^n\omega^{2n}\beta^{2n}\ , \qquad (5.16)$$

where the last term on the right-hand side is absent when $n=0$. Note that because of the very simple variable dependence on the factor θ in Eq. (5.13) for L_n, it turns out that the series for L_n, W_n, and S_n are essentially the same series and have a common radius of convergence. This special situation will not characterize the general problem.

The formulas (5.14), (5.15), and (5.16) may be compared with their diagonal ($\vec{x}=\vec{x}\,'$) counterparts in Sec. IV. Complete agreement is found. This check is satisfactory, since our linked-graph method provides the correct result for the first several coefficient functions. Nevertheless, it is of greater interest to show how the general result (5.13) for L_l emerges from the solution of Sec. IV.

Consider the value of L_l implied by its linked-graph form. The values of L_1 and L_2 are elementary and follow directly from their definition in formulas (4.1) and (4.2) after the substitution $v(\vec{x})=\frac{1}{2}m\omega^2\vec{x}^2$. So take $l\geq 3$. The general form of L_l is

$$L_l(\vec{x},\vec{x}\,';\beta,q)=\frac{1}{l!}\int_0^1\cdots\int_0^1 d\xi_1\cdots d\xi_l\times F(a)f_1\cdots f_2\ , \qquad (5.17)$$

where f_i are defined by Eq. (3.2). $F(a)$ is a polynomial of the a_{ij} that appear in Eq. (3.5). The structure of the polynomial is determined by the definition of the sum of all distinct l-vertex linked graphs that can enter L_l. The a_{ij} contains powers of the derivatives of $\vec{\nabla}_i$ and $\vec{\nabla}_j$. Since $v(\vec{x})$ is quadratic in $\vec{x}$, so is f_i. Thus each vertex i can have at most two links attached to it. A three-link vertex would have third-order derivatives of a quadratic form in $\vec{x}$ and thus be zero. The only nonvanishing linked graphs in L_l are those formed of two- and one-linked vertices. Within this restriction, there are only two topologically distinct graph structures. Type I is that formed of $l-1$ links. It has two vertices with one link with all other vertices having two links. Type II has l links; here every vertex has two links. If the vertices are arranged to be equally spaced along the perimeter of a circle, then type-II graphs appear as an l-sided polygon. On the other hand, type-I graphs appear as an l-sided polygon with one side missing. The type-II graphs are the ring graphs discussed by Montroll and Ward.[16]

The two distinct topological graphs types let us decompose L_l as

$$L_l=L_l^{(\mathrm{I})}+L_l^{(\mathrm{II})} \quad (l\geq 3)\ . \tag{5.18}$$

The f_i that enter L_l can be replaced by $-\beta v_i$, since the higher powers of β in f_i all lead to zero. Keeping in mind that the permutation of the labels $1,2,\ldots,l$ lead to $l!/2$ distinct graphs of type I and $(l-1)!/2$ distinct graphs of type II, we can write

$$L_l^{(\mathrm{I})}=\frac{(-\beta)^l}{l!}\frac{l!}{2}\int_0^1 d\xi_1\cdots\int_0^1 d\xi_l a_{12}a_{23}\cdots a_{l-1,l} \times v_1\cdots v_l\ , \tag{5.19}$$

$$L_l^{(\mathrm{II})}=\frac{(-\beta)^l}{l!}\frac{(l-1)!}{2} \times\int_0^1 d\xi_1\cdots\int_0^1 d\xi_l a_{12}\cdots a_{l-1,l}a_{1,l}v_1\cdots v_l\ . \tag{5.20}$$

Substituting the harmonic-oscillator form of the potential gives

$$L_l^{(\mathrm{I})}=\frac{(-\beta)^l}{2}(2\gamma)^{l-1}\left[\frac{m\omega^2}{2}\right]^l \times\int_0^1 d\xi_1\cdots\int_0^1 d\xi_l\Phi_{1,l}J_{1,l}\big|_{\vec{x}_i=\hat{\xi}_i}\ , \tag{5.21}$$

$$L_l^{(\mathrm{II})}=\frac{(-\beta)^l}{2l}(2\gamma)^l\left[\frac{m\omega^2}{2}\right]^l \times\int_0^1 d\xi_1\cdots\int_0^1 d\xi_l\Phi_{1,l}\phi_{1,l}(\vec{\nabla}_1\cdot\vec{\nabla}_l)J_{1,l}\ , \tag{5.22}$$

where

$$\Phi_{1,l}=\phi_{12}\phi_{23}\phi_{34}\cdots\phi_{l-1,l}\ , \tag{5.23}$$

$$\phi_{ij}=\phi(\xi_i,\xi_j)=\xi_<(1-\xi_>)\ , \tag{5.24}$$

$$J_{1,l}=(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\nabla}_2\cdot\vec{\nabla}_3)\cdots(\vec{\nabla}_{l-1}\cdot\vec{\nabla}_l)\vec{x}_1^2\cdots\vec{x}_l^2 \tag{5.25}$$

From the definition of $J_{1,l}$, a little algebra shows that

$$J_{1,l}=2^l\vec{x}_1\cdot\vec{x}_l\ , \tag{5.26}$$

and

$$(\vec{\nabla}_1\cdot\vec{\nabla}_l)J_{1,l}=3N\,2^l\ . \tag{5.27}$$

Upon using the identity

$$\vec{x}_1\cdot\vec{x}_l\big|_{\vec{x}_i=\hat{\xi}_i}=(1-\xi_1)(1-\xi_l)\vec{x}^2+\xi_1\xi_l\vec{x}'^2 +(\xi_1+\xi_l-2\xi_1\xi_l)\vec{x}\cdot\vec{x}'\ , \tag{5.28}$$

we see that the $L_l^{(\mathrm{I})}$ and $L_l^{(\mathrm{II})}$ may be written

$$L_l^{(\mathrm{I})}=(-\beta)^l\tfrac{1}{2}(2\gamma)^{l-1}(m\omega^2)^l \times[(\vec{x}^2+\vec{x}'^2)I_1+\vec{x}\cdot\vec{x}'(2I_2-2I_1)]\ , \tag{5.29}$$

$$L_l^{(\mathrm{II})}=(-\beta)^l\frac{1}{2l}(2\gamma)^l(m\omega^2)^l 3N\mathrm{I}_0\ . \tag{5.30}$$

The three integrals I_i are

$$I_0=\int_0^1 d\xi_1\cdots\int_0^1 d\xi_l\Phi_{1,l}\phi_{1,l}\ ,$$
$$I_1=\int_0^1 d\xi_1\cdots\int_0^1 d\xi_l\xi_1\xi_l\Phi_{1,l}\ , \tag{5.31}$$
$$I_2=\int_0^1 d\xi_1\cdots\int_0^1 d\xi_l\xi_1\Phi_{1,l}\ .$$

Comparing (5.29) and (5.30) with (5.13), it is apparent that the general form of L_l is correctly determined.

The last step is to understand how the Bernoulli numbers emerge from I_i, $i=0,1,2$. In order to carry out the I_i integrals explicitly, recall that $\phi(\xi,\xi')=\xi_<(1-\xi_>)$ is the Green's function for the one-dimensional eigenvalue problem

$$-\frac{d^2}{dy^2}\psi(y)=\lambda\psi(y)\ , \tag{5.32}$$

with boundary condition $\psi(0)=\psi(1)=0$. The solution has eigenvalues $\lambda_n=(n\pi)^2$ $(n=1,2,\ldots)$ and associated eigenfunctions

$$\psi_n(y)=\sqrt{2}\sin n\pi y \ . \tag{5.33}$$

Thus, by Mercer's theorem,[17] the Green's function has the representation

$$\phi(\xi,\xi')=\xi_<(1-\xi_>)=\sum_{n=1}^{\infty}\frac{\Psi_n(\xi)\Psi_n(\xi')}{\lambda_n} ,$$
$$=\sum_{n=1}^{\infty}\frac{2\sin n\pi\xi\,\sin n\pi\xi'}{(\pi n)^2} \ . \tag{5.34}$$

Now, if expansion (5.34) is used for all the ϕ_{ij} in I_0, the mutual orthogonality of all the eigenfunctions $\Psi_n(\xi_i)$ permits one to find

$$I_0=\sum_{n=1}^{\infty}\frac{1}{\lambda_n^l}=(-1)^{l-1}\frac{2^{2l-1}}{(2l)!}B_{2l} , \tag{5.35}$$

where the right-hand side equality uses the Bernoulli number definition (5.8). Similarly, one finds

$$I_1=2I_0 \ , \quad I_2=\left[4-\frac{1}{2^{2l-2}}\right]I_0 \ . \tag{5.36}$$

Inserting these values of I_i into (5.29) and (5.30) leads exactly to Eq. (5.13) for L_l. So we have demonstrated that the linked-graph method leads to a construction of the known closed-form solution for L_l in the harmonic-oscillator problem.

VI. CONCLUSIONS

The Wigner-Kirkwood semiclassical expansion of the quantum-partition function is one of the oldest semiclassical expansions in the literature. Although the first few terms of this type of expansion of $F(\vec{x},\vec{x}\,';\beta,q)$ have been derived in a number of different ways, no systematic method for obtaining the explicit functional form of an arbitrary coefficient $S_n(\vec{x},\vec{x}\,';\beta)$ has been available. The problem of determining the coefficient functions for the β- and q-power-series expansions of $\ln F(\vec{x},\vec{x}\,';\beta,q)$ is solved in Secs. II–IV. By using the Goldberger-Adams representation of $F(\vec{x},\vec{x}\,';\beta,q)$, we showed that the series expansion of F in the coupling constant α may be given in a form that has the same combinatorial structure as one finds for the grand canonical partition function in classical statistical mechanics. Thus, it is possible to exponentiate the coupling-constant expansion for F. In this fashion, the α-series expansion for $\ln F$ is given by coefficient functions which are computed from a sum of linked graphs. Reexpanding the linked graphs in the variables q and β give one explicit formulas for the functions $S_n(\vec{x},\vec{x}\,';\beta)$ and $W_n(\vec{x},\vec{x}\,';q)$. The solution described here is of a rather general character. It succeeds for any number of particles and gives coefficient functions valid on $(\vec{x}\,'=\vec{x})$ and off $(\vec{x}\,'\neq\vec{x})$ diagonal. The Appendix shows how the solution described above results if one employs path-integral techniques in place of the Goldberger-Adams representation.

APPENDIX: PATH-INTEGRAL REPRESENTATIONS OF THE PARTITION FUNCTION

This appendix extends our analysis of $F(\vec{x},\vec{x}\,';\beta,q)$ by incorporating the path-integral description of the partition function. By starting from the Goldberger-Adams representation, it will be shown that it is a simple matter to derive the functional-integral form $F(\vec{x},\vec{x}\,';\beta,q)$. This functional-integral form provides us with a Feynman-Kac-type path-integral representation of F. Further, assuming the path-integral representation of F as given, we show how it is possible to derive the basic identity of Sec. II, Eq. (2.27). The results of this appendix are of interest because they provide an additional perspective on the representations given in Sec. II. Also, we believe, the functional-integral forms are most likely to be the simplest way to enlarge the physical framework of this theory in order to include the effects of spin, relativity, and symmetrization of identical particles.

The Goldberger-Adams formula for $F(\vec{x},\vec{x}\,';\beta,q)$, Eq. (2.16), reads, after an obvious change of variables,

$$\langle\vec{x}\,|\,e^{-\beta H}\,|\,\vec{x}\,'\rangle=\langle\vec{x}\,|\,e^{-\beta H_0}\,|\,\vec{x}\,'\rangle \times\exp_<\left[-\int_0^{\beta}d\beta' v\left[\vec{x}\,'+\frac{\beta'}{\beta}(\vec{x}-\vec{x}\,')+2q\beta'\vec{\nabla}_{x'}\right]\right]1 \ . \tag{A1}$$

Consider the form of Eq. (A1) when the value of β is small. For a well-behaved potential (for example, one which is smooth and uniformly bounded with respect to any order of derivatives), then (A1) implies

$$\langle \vec{x} \,|\, e^{-\Delta\beta H} \,|\, \vec{x}\,' \rangle = \langle \vec{x} \,|\, e^{-\Delta\beta H_0} \,|\, \vec{x}\,' \rangle \exp\left[-\int_0^{\Delta\beta} d\beta' v \left[\vec{x}\,' + \frac{\beta'}{\Delta\beta}(\vec{x}-\vec{x}\,') \right] + O((\Delta\beta)^2) \right] , \tag{A2}$$

for $\Delta\beta \sim 0$. Discretize the description here, by dividing the finite interval $(0,\beta)$ into n equal segments for an arbitrary n; $\Delta\beta \equiv \beta n^{-1}$ and $\beta_i \equiv i\Delta\beta (i=0\sim n)$. Then using the semigroup property of $e^{-\beta H}$, we get

$$\begin{aligned} \langle \vec{x} \,|\, e^{-\beta H} \,|\, \vec{x}\,' \rangle &= \langle \vec{x} \,|\, (e^{-H\Delta\beta})^n \,|\, \vec{x}\,' \rangle \\ &= \int d\vec{x}_1 \cdots \int d\vec{x}_{n-1} \langle \vec{x} \,|\, e^{-H\Delta\beta} \,|\, \vec{x}_{n-1} \rangle \langle \vec{x}_{n-1} \,|\, e^{-H\Delta\beta} \,|\, \vec{x}_{n-2} \rangle \cdots \langle \vec{x}_1 \,|\, e^{-H\Delta\beta} \,|\, \vec{x}\,' \rangle \\ &= \int d\vec{x}_1 \cdots \int d\vec{x}_{n-1} \langle \vec{x} \,|\, e^{-H_0\Delta\beta} \,|\, \vec{x}_{n-1} \rangle \cdots \langle \vec{x}_1 \,|\, e^{-H_0\Delta\beta} \,|\, \vec{x}\,' \rangle \\ &\quad \times \exp\left[-\sum_{i=0}^{n-1} \int_0^{\Delta\beta} d\tilde{\beta}\, v \left[\vec{x}_i + \frac{\tilde{\beta}}{\Delta\beta}(\vec{x}_{i+1}-\vec{x}_i) \right] + O(n(\Delta\beta)^2) \right] . \end{aligned} \tag{A3}$$

Introduce the broken line path defined by

$$\vec{x}_n(\tilde{\beta}) = \vec{x}_i + \left[\frac{\tilde{\beta}}{\Delta\beta} - i \right] (\vec{x}_{i+1}-\vec{x}_i) \quad \text{for } \beta_i \le \tilde{\beta} < \beta_{i+1} , \tag{A4}$$

where $i=0\sim n-1$. The end points are $\vec{x}_0 \equiv \vec{x}\,'$ and $\vec{x}_n \equiv \vec{x}$. With this notation, the sum of integrals in the exponential of (A3) is written as $-\int_0^{\beta} d\tilde{\beta}\, v[\vec{x}_n(\tilde{\beta})]$. On the other hand, by Eq. (2.11), we see that the product of the n free heat kernels is

$$(4\pi q \Delta\beta)^{-n\delta} \exp\left[-\sum_{i=0}^{n-1} \frac{(\vec{x}_{i+1}-\vec{x}_i)^2}{4q\Delta\beta} \right] . \tag{A5}$$

Recall that δ is the dimension of x divided by 2. In this way, (A3) can be represented by

$$\begin{aligned} \langle \vec{x} \,|\, e^{-\beta H} \,|\, \vec{x}\,' \rangle = (4\pi q \Delta\beta)^{-n\delta} \int d\vec{x}_1 \cdots \int d\vec{x}_{n-1} \exp\left[-\sum_{i=0}^{n-1} \frac{(\vec{x}_{i+1}-\vec{x}_i)^2}{4q\Delta\beta} \right] \\ \times \exp\left[-\int_0^{\beta} d\tilde{\beta}\, v[\vec{x}_n(\tilde{\beta})] + O(n(\Delta\beta)^2) \right] . \end{aligned} \tag{A6}$$

Letting $n \to \infty$ recovers the path-integral expression for the heat kernel,

$$\begin{aligned} \langle \vec{x} \,|\, e^{-\beta H} \,|\, \vec{x}\,' \rangle = \lim_{n\to\infty} (4\pi q \Delta\beta)^{-n\delta} \int d\vec{x}_1 \cdots \int d\vec{x}_{n-1} \exp\left[-\sum_{i=0}^{n-1} \frac{(\vec{x}_{i+1}-\vec{x}_i)^2}{4q\Delta\beta} \right] \\ \times \exp\left[-\int_0^{\beta} d\tilde{\beta}\, v[\vec{x}_n(\tilde{\beta})] \right] , \end{aligned} \tag{A7}$$

$$\langle \vec{x} \,|\, e^{-\beta H} \,|\, \vec{x}\,' \rangle \equiv \langle \vec{x} \,|\, e^{-\beta H_0} \,|\, \vec{x}\,' \rangle \int_{C(0,\vec{x}\,';\beta,\vec{x})} d^{*}_{w(0,\vec{x}\,';\beta,\vec{x})}\vec{x} \exp\left[-\int_0^{\beta} d\tilde{\beta}\, v[\vec{x}(\tilde{\beta})] \right] . \tag{A8}$$

In Eq. (A8), the integral notation indicates the conditional Wiener measure. The space of all continuous paths $\vec{x}(\tilde{\beta})$ satisfying the condition $\vec{x}(0)=\vec{x}\,'$ and $\vec{x}(\beta)=\vec{x}$ is denoted by $C(0,\vec{x}\,';\beta,\vec{x})$. The conditional Wiener measure has the normalization

$$\int_{C(0,\vec{x}\,';\beta,\vec{x})} d^{*}_{w(0,\vec{x}\,';\beta,\vec{x})}\vec{x} = 1 . \tag{A9}$$

For a detailed discussion of these Wiener measures, see papers of Yaglom[13] and Gelfand and Yaglom.[18] Equation (A8) is a variant[19] of the one that Kac[20] showed is the solution of the heat equation (2.28) that satisfies the delta-function boundary condition (2.29). It is interesting to note that recent work by Truman[21] shows that the limit (A7) exists for a very wide class of potentials even when the Wiener measure is replaced by the more intractable "Feynman measure."

Consider next a change of variables that will further simplify the functional integral (A8). Define a new broken line path by

$$\vec{x}_i \to \vec{y}_i = \vec{x}_i - \vec{\eta}(\beta_i) \quad (i = 0 \sim n) \tag{A10}$$

where

$$\vec{\eta}(\tilde{\beta}) = \vec{x}\,' + \frac{\tilde{\beta}}{\beta}(\vec{x} - \vec{x}\,') = \frac{\tilde{\beta}}{\beta}\vec{x} + \left[1 - \frac{\tilde{\beta}}{\beta}\right]\vec{x}\,' . \tag{A11}$$

Clearly the y-variable end points are $\vec{y}_0 = \vec{y}_n = 0$. A short calculation shows that

$$\vec{x}_n(\tilde{\beta}) = \vec{y}_n(\tilde{\beta}) + \vec{\eta}(\tilde{\beta}) , \tag{A12}$$

where $\vec{y}_n(\tilde{\beta})$ is Eq. (A4) with $\vec{x}_i \to \vec{y}_i$ on the right-hand side. One also finds

$$\sum_{i=0}^{n-1} (\vec{x}_{i+1} - \vec{x}_i)^2 = \sum_{i=0}^{n-1} (\vec{y}_{i+i} - \vec{y}_i)^2 + \frac{1}{n}(\vec{x} - \vec{x}\,')^2 . \tag{A13}$$

If we substitute (A12) and (A13) into (A6) and then let $n \to \infty$, we get, after replacing $\vec{y}$ with $\vec{x}$,

$$F(\vec{x},\vec{x}\,';\beta,q) = \lim_{n\to\infty} (4\pi\beta q)^{\delta}(4\pi q\Delta\beta)^{-n\delta} \int d\vec{x}_1 \cdots \int d\vec{x}_{n-1} \exp\left[-\sum_{i=0}^{n-1} \frac{(\vec{x}_{i+1} - \vec{x}_i)^2}{4q\Delta\beta}\right] \times \exp\left[-\int_0^\beta d\tilde{\beta}\, v[\vec{\eta}(\tilde{\beta}) + \vec{x}_n(\tilde{\beta})]\right]$$

$$= \int_{C(\beta,0)} d^*_{w(\beta,0)}\vec{x} \exp\left[-\int_0^\beta d\tilde{\beta}\, v[\vec{\eta}(\tilde{\beta}) + \vec{x}(\tilde{\beta})]\right] , \tag{A14}$$

where $\vec{x}_0 = \vec{x}_n = 0$. The measure notation in (A14) denotes the conditional measure defined by $C(\beta,0) \equiv C(0,0;\beta,0)$ and $d^*_{w(\beta,0)}\vec{x} = d^*_{w(0,0;\beta,0)}\vec{x}$.

The remainder of this appendix is devoted to obtaining a path-integral derivation of the key identity, Eq. (2.27). Begin with (A14) and the Taylor expansion

$$v[\vec{\eta}(\tilde{\beta}) + \vec{x}(\tilde{\beta})] = e^{\vec{x}(\tilde{\beta})\cdot\vec{\nabla}} v[\vec{\eta}(\tilde{\beta})] , \tag{A15}$$

where $\vec{\nabla}$ acts on v. Assuming the interchangeability of the sum and integrals (A14) becomes

$$F = \int_{C(\beta,0)} d^*_{w(\beta,0)}\vec{x} \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \left[\int_0^\beta d\tilde{\beta}\, v[\vec{\eta}(\tilde{\beta}) + \vec{x}(\tilde{\beta})]\right]^l$$

$$= \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \int_0^\beta d\tilde{\beta}_1 \cdots \int_0^\beta d\tilde{\beta}_l \int_{C(\beta,0)} d^*_{w(\beta,0)}\vec{x} \exp\left[\sum_{\mu=1}^{l} \vec{x}(\tilde{\beta}_\mu)\cdot\vec{\nabla}_\mu\right] v[\vec{\eta}(\tilde{\beta}_1)] \cdots v[\vec{\eta}(\tilde{\beta}_l)] . \tag{A16}$$

We will prove subsequently, for any arbitrary 2δ-dimensional vectors $\vec{a}_1, \ldots, \vec{a}_l$ and $0 \le \tilde{\beta}_1 \le \cdots \le \tilde{\beta}_l \le \beta$, that

$$\int_{C(\beta,0)} d^*_{w(\beta,0)}\vec{x} \exp\left[\sum_{\mu=1}^{l} \vec{x}(\tilde{\beta}_\mu)\cdot\vec{a}_\mu\right] = \exp\left[q \sum_{\mu,\nu=1}^{l} G(\tilde{\beta}_\mu,\tilde{\beta}_\nu)\vec{a}_\mu\cdot\vec{a}_\nu\right] , \tag{A17}$$

where $\tilde{\beta}_< \equiv \min\{\tilde{\beta},\tilde{\beta}'\}, \tilde{\beta}_> \equiv \max\{\tilde{\beta},\tilde{\beta}'\}$ and G is defined as

$$G(\tilde{\beta},\tilde{\beta}') = \frac{\tilde{\beta}_<(\beta - \tilde{\beta}_>)}{\beta} . \tag{A18}$$

Utilizing identity (A17) in Eq. (A16) lets us write

$$F = \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \int_0^\beta d\tilde{\beta}_1 \cdots \int_0^\beta d\tilde{\beta}_l \exp\left[q \sum_{\mu,\nu=1}^{l} G(\tilde{\beta}_\mu,\tilde{\beta}_\nu)\vec{\nabla}_\mu\cdot\vec{\nabla}_\nu\right] v[\vec{\eta}(\tilde{\beta}_1)] \cdots v[\vec{\eta}(\tilde{\beta}_l)] . \tag{A19}$$

Equation (A19) is essentially Eq. (2.27). To see this, employ the invariance of F under $\vec{x}\leftrightarrow\vec{x}\,'$ and make the replacement $\tilde{\beta}_i\to\xi_i$ by $\tilde{\beta}_i=\beta\xi_i$.

According to the pseudomeasure approach developed by DeWitt-Morette,[22] the Feynman integral, Eq. (A17), is a special value of the Fourier transform of the Wiener measure which has both end points fixed. However, we can establish Eq. (A17) in a straightforward manner starting from the simple definition of Wiener measure given in Eq. (A14). We sketch the proof here for completeness. The technique we use is the one already employed in I in order to study the Born series.

First consider a prototype of the integral in (A17). Take K to be any well-behaved function of $\vec{x}$, then define

$$I_n\equiv(4\pi\beta q)^{\delta}(4\pi q\Delta\beta)^{-n\delta}\int d\vec{x}_1\cdots\int d\vec{x}_{n-1}\exp\left[-\sum_{i=0}^{n-1}\frac{(\vec{x}_{i+1}-\vec{x}_i)^2}{4q\Delta\beta}\right]K[\bar{x}_n(\tilde{\beta})]\,, \tag{A20}$$

where $\vec{x}_0=\vec{x}_n=0$. Use the formula

$$\sum_{i=0}^{n-1}(\vec{x}_{i+1}-\vec{x}_i)^2=\sum_{i=1}^{n-1}\frac{\beta-\beta_{i-1}}{\beta-\beta_i}\left[\vec{x}_i-\frac{\beta-\beta_i}{\beta-\beta_{i-1}}\vec{x}_{i-1}\right]^2, \tag{A21}$$

where $\beta_i=i\Delta\beta(i=0\sim n)$ with $\Delta\beta=\beta/n$ and $\vec{x}_0=\vec{x}_n=0$. Now make the variable change

$$\vec{y}_i\,'=\vec{x}_i-\frac{\beta-\beta_i}{\beta-\beta_{i-1}}\vec{x}_{i-1}\quad(i=1\sim n-1)\,. \tag{A22}$$

The inverse of (A22) is found to be

$$\vec{x}_i=\sum_{j=1}^{i}\frac{\beta-\beta_i}{\beta-\beta_j}\vec{y}_j\,'\quad(i=1\sim n-1)\,. \tag{A23}$$

This transformation causes the broken path to be represented by

$$\bar{x}_n(\tilde{\beta})=(\beta-\tilde{\beta})\sum_{j=1}^{i}\frac{1}{\beta-\beta_j}\vec{y}_j\,'+\frac{\tilde{\beta}-\beta_i}{\Delta\beta}\vec{y}_{i+1}\,'\,, \tag{A24}$$

for $\beta_i\le\tilde{\beta}<\beta_{i+1}$. Finally, a scale change is introduced by

$$\vec{y}_i=\frac{1}{(4q\Delta\beta)^{1/2}}\left[\frac{\beta-\beta_{i-1}}{\beta-\beta_i}\right]^{1/2}\vec{y}_i\,'\quad(i=1\sim n-1)\,. \tag{A25}$$

The combined change of variables (A22) and (A25) has a Jacobian given by

$$d\vec{x}_1\cdots d\vec{x}_{n-1}=(4q\beta)^{-\delta}(4q\Delta\beta)^{n\delta}d\vec{y}_1\cdots d\vec{y}_{n-1}\,, \tag{A26}$$

and so I_n is rewritten as

$$I_n=\left[\prod_{k=1}^{n-1}\pi^{-\delta}\int d\vec{y}_k e^{-\vec{y}_k^{\,2}}\right]K\left\{\sqrt{4q}\left[(\beta-\tilde{\beta})\sum_{j=1}^{i}\left[\frac{1}{\beta-\beta_j}-\frac{1}{\beta-\beta_{j-1}}\right]^{1/2}\vec{y}_j\right.\right.$$
$$\left.\left.+(\tilde{\beta}-\beta_i)\left[\frac{1}{\Delta\beta}-\frac{1}{\beta-\beta_i}\right]^{1/2}\vec{y}_{i+1}\right]\text{ for }\beta_i\le\tilde{\beta}<\beta_{i+1}\right\}. \tag{A27}$$

In Eq. (A27), it is understood that the requirement $\beta_i\le\tilde{\beta}<\beta_{i+1}$ selects the value of i. In this way, i is to be interpreted as a function of β; where $i=[\tilde{\beta}/\Delta\beta]$ with $[\cdot]$ being the integer part.

Let's generalize $K[\bar{x}_n(\beta)]$ to the form occurring in (A17),

$$K[\bar{x}_n(\tilde{\beta}_1),\ldots,\bar{x}_n(\tilde{\beta}_l)]=\exp\left[\sum_{\mu=1}^{l}\bar{x}_n(\tilde{\beta}_\mu)\cdot\vec{a}_\mu\right]. \tag{A28}$$

In the case of the function K in (A28) with l different path arguments $(\tilde{\beta}_1,\tilde{\beta}_2,\ldots,\tilde{\beta}_l)$ each value of $\tilde{\beta}_\mu$ will select a value of i for example, (i_μ) so that $\beta_{i_\mu} \le \tilde{\beta}_\mu \le \beta_{i_\mu+1}$ $(\mu=1\sim l)$. Thus the right-hand side of (A28) becomes, when it is placed in (A27),

$$\exp\left\{\sum_{\mu=1}^{l}\sqrt{4q}\left[(\beta-\tilde{\beta}_\mu)\sum_{j=1}^{i_\mu}\left[\frac{1}{\beta-\beta_j}-\frac{1}{\beta-\beta_{j-1}}\right]^{1/2}\vec{y}_j+(\tilde{\beta}_\mu-\beta_{i_\mu})\left[\frac{1}{\Delta\beta}-\frac{1}{\beta-\beta_{i_\mu}}\right]^{1/2}\vec{y}_{i_\mu+1}\right]\cdot\vec{a}_\mu\right\}$$

$$=\exp\left[\sqrt{4q}\sum_{j=1}^{n-1}\vec{A}_j\cdot\vec{y}_j\right], \qquad (A29)$$

where the vector $\vec{A}_j$ is

$$\vec{A}_j\equiv\left[\frac{1}{\beta-\beta_j}-\frac{1}{\beta-\beta_{j-1}}\right]^{1/2}\sum_{\mu=1}^{l}\Theta(i_\mu-j)(\beta-\tilde{\beta}_\mu)\vec{a}_\mu+\sum_{\mu=1}^{l}\delta_{j,i_\mu+1}\left[\frac{1}{\Delta\beta}-\frac{1}{\beta-\beta_{i_\mu}}\right]^{1/2}(\tilde{\beta}_\mu-\beta_{i_\mu})\vec{a}_\mu \qquad (A30)$$

for $j=1\sim n-1$. Here Θ is the Heaviside function, $\Theta(x)=1$ if $x\ge 0$ and otherwise is zero. The purpose of the elaborate variable changes in (A22) and (A25) is to reduce the integral I_n into a product of simple Gaussian integrals, each of which is trivial to compute. Using (A29) gives us this desired form

$$I_n=\prod_{j=1}^{n-1}\left[\pi^{-\delta}\int d\vec{y}_j\exp(-\vec{y}_j^{\,2}+\sqrt{4q}\,\vec{A}_j\cdot\vec{y}_j)\right]=\prod_{j=1}^{n-1}\exp(q\vec{A}_j^{\,2})=\exp\left[q\sum_{j=1}^{n-1}\vec{A}_j^{\,2}\right]. \qquad (A31)$$

Calculating the value of the argument of the last exponential gives us

$$\sum_{j=1}^{n-1}\vec{A}_j^{\,2}=\sum_{\mu,\nu=1}^{l}\vec{a}_\mu\cdot\vec{a}_\nu\left[\frac{(\beta-\tilde{\beta}_\mu)(\beta-\tilde{\beta}_\nu)\beta_{i_\mu\wedge i_\nu}}{\beta(\beta-\beta_{i_\mu\wedge i_\nu})}+2\Theta(i_\mu-i_\nu-1)\frac{(\beta-\tilde{\beta}_\mu)(\tilde{\beta}_\nu-\beta_{i_\nu})}{\beta-\beta_{i_\nu}}\right.$$
$$\left.+\,\delta_{i_\mu,i_\nu}\frac{(\tilde{\beta}_\mu-\beta_{i_\mu})(\tilde{\beta}_\nu-\beta_{i_\nu})(\beta-\beta_{i_\mu+1})}{\Delta\beta(\beta-\beta_{i_\mu})}\right], \qquad (A32)$$

where $i_\mu\wedge i_\nu$ denotes the least value of i_μ and i_ν. The last step of our calculation is to let $n\to\infty$. Recalling the definition of i_μ we have that

$$\beta_{i_\mu},\beta_{i_\mu+1}\to\tilde{\beta}_\mu \quad (\mu=1\sim l)\,. \qquad (A33)$$

Thus only the first term of $(\cdots)$ in (A32) survives and gives $G(\tilde{\beta}_\mu,\tilde{\beta}_\nu)$ as defined in (A18). Thus, altogether, we get

$$\lim_{n\to\infty} I_n=\exp\left[q\sum_{\mu,\nu=1}^{l}G(\tilde{\beta}_\mu,\tilde{\beta}_\nu)\vec{a}_\mu\cdot\vec{a}_\nu\right]. \qquad (A34)$$

This completes the proof of identity (A17).

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